



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:35 am BST

PDB ID : 2QKY  
Title : complex structure of dipeptidyl peptidase IV and a oxadiazolyl ketone  
Authors : Kim, K.-H.; Hong, S.Y.; Koo, K.D.; Lee, C.-S.; Kim, G.T.; Han, H.O.  
Deposited on : 2007-07-12  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

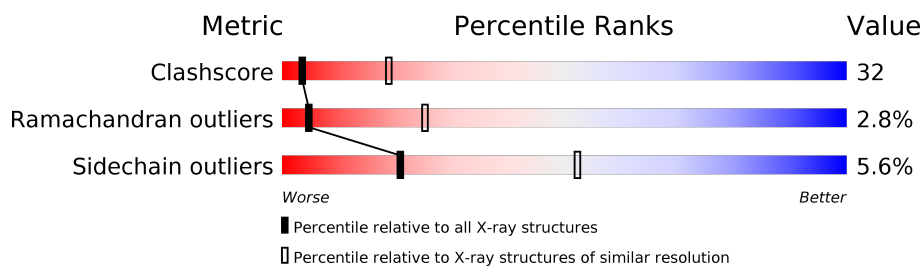
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div>44%</div> <div>51%</div> <div>5%</div> </div>
1	B	728	<div> <div>46%</div> <div>49%</div> <div>.</div> </div>
1	C	728	<div> <div>46%</div> <div>49%</div> <div>5%</div> </div>
1	D	728	<div> <div>47%</div> <div>48%</div> <div>5%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24275 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

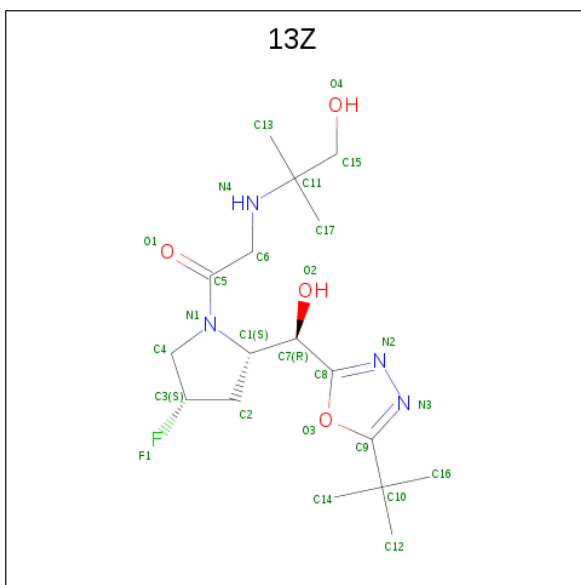
- Molecule 1 is a protein called Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	B	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	C	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	D	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	-	EXPRESSION TAG	UNP P27487
B	39	THR	-	EXPRESSION TAG	UNP P27487
C	39	THR	-	EXPRESSION TAG	UNP P27487
D	39	THR	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is 2-[(2-{(2S,4S)-2-[(R)-(5-tert-butyl-1,3,4-oxadiazol-2-yl)(hydroxy)methyl]-4-fluoropyrrolidin-1-yl}-2-oxoethyl)amino]-2-methylpropan-1-ol (three-letter code: 13Z) (formula: C<sub>17</sub>H<sub>29</sub>FN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	B	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	C	1	Total 26	C 17	F 1	N 4	O 4	0	0
2	D	1	Total 26	C 17	F 1	N 4	O 4	0	0

- Molecule 3 is water.

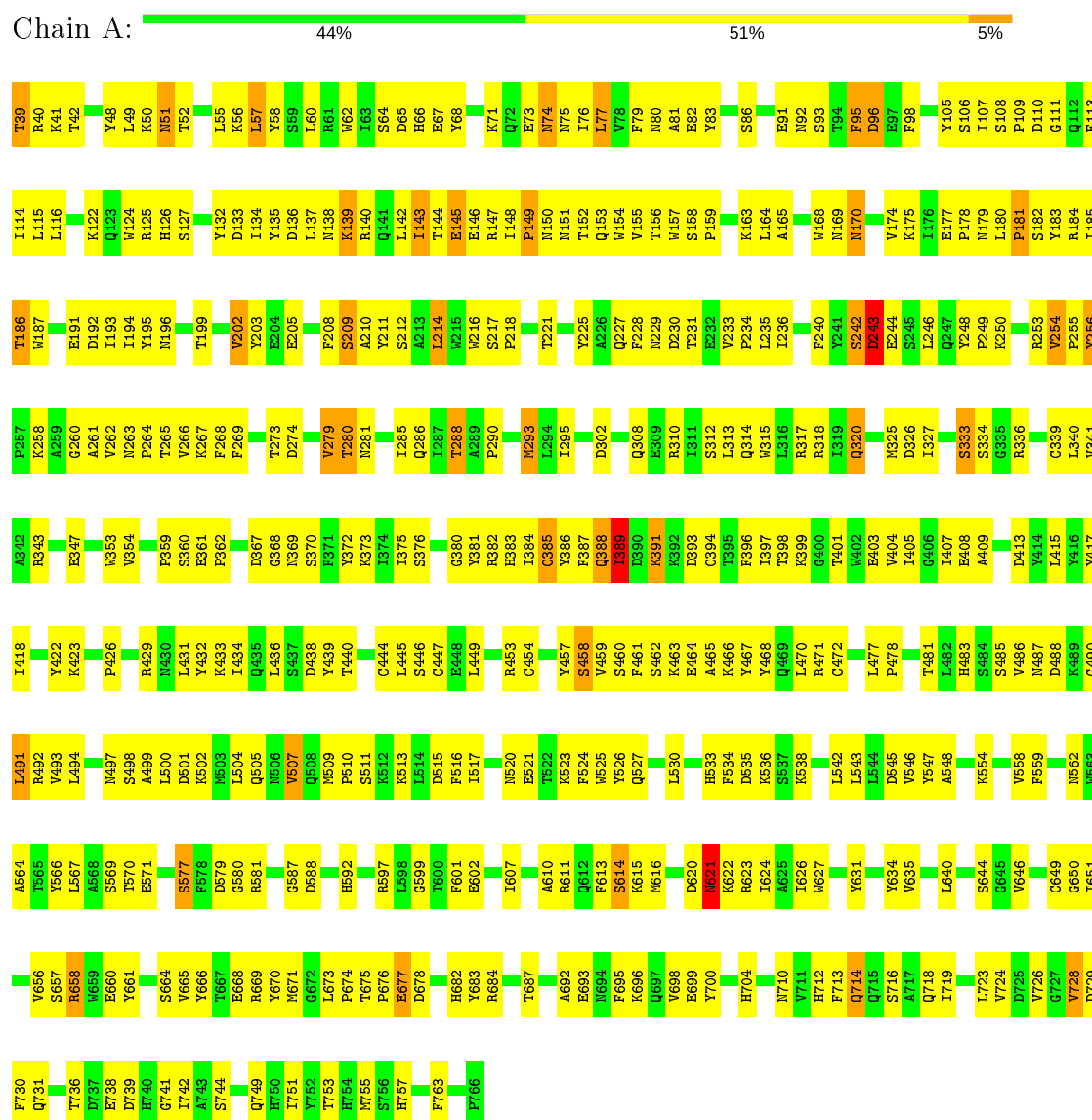
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	72	Total	O	0	0
			72	72		
3	C	66	Total	O	0	0
			66	66		
3	D	92	Total	O	0	0
			92	92		

### 3 Residue-property plots

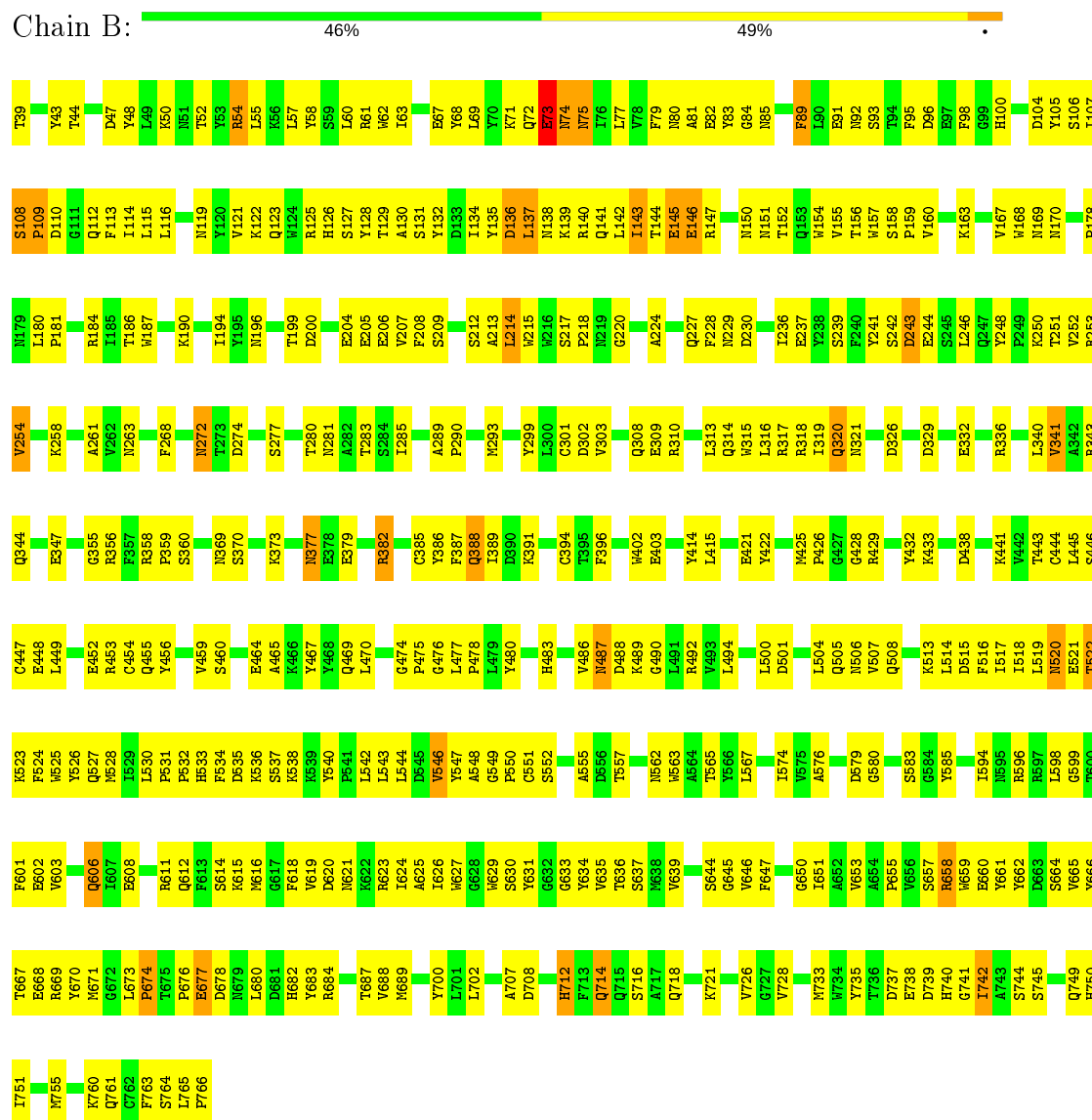
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

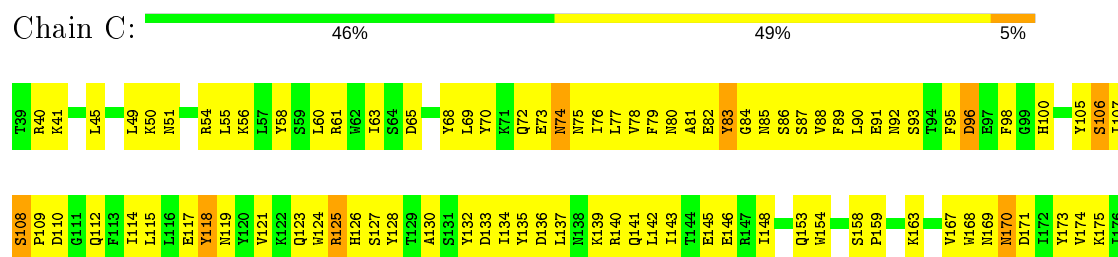
- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

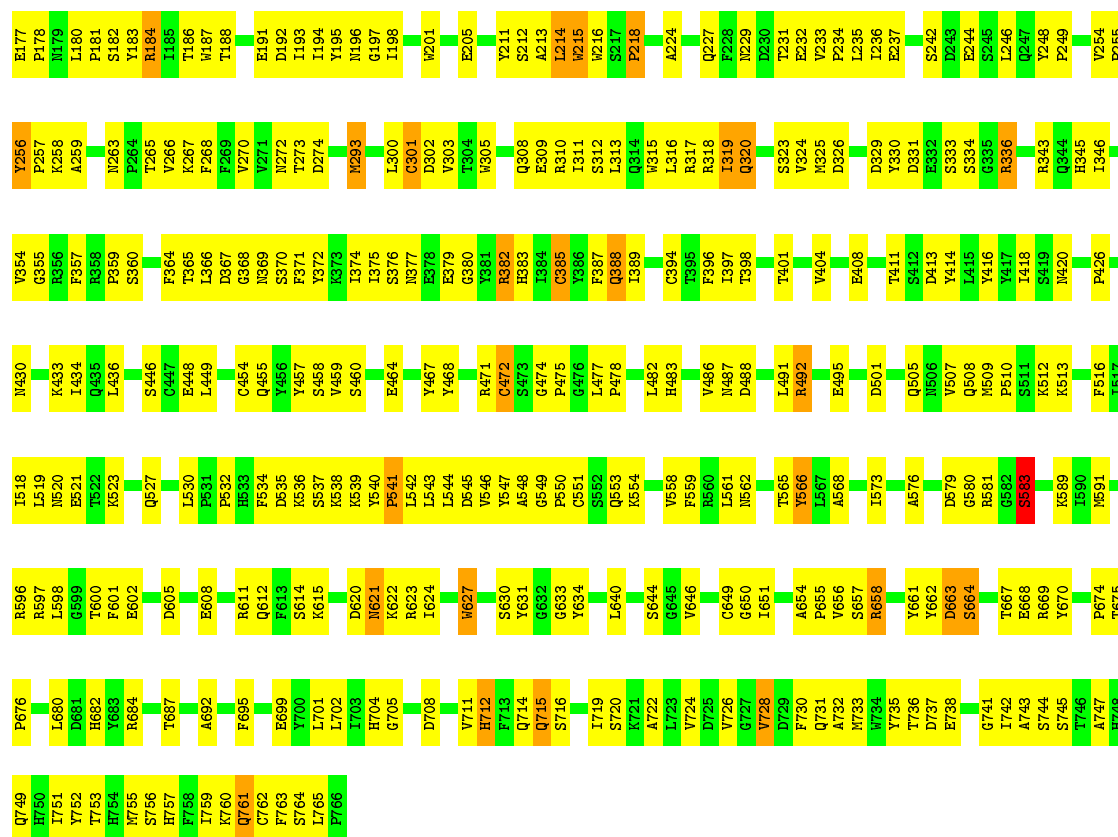


- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)



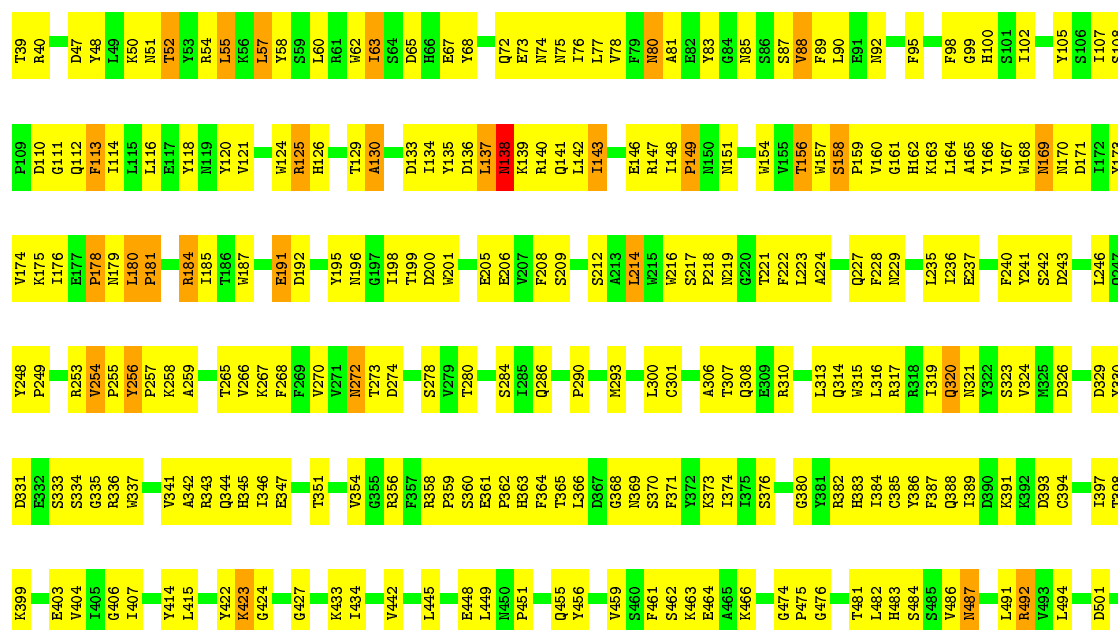
- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

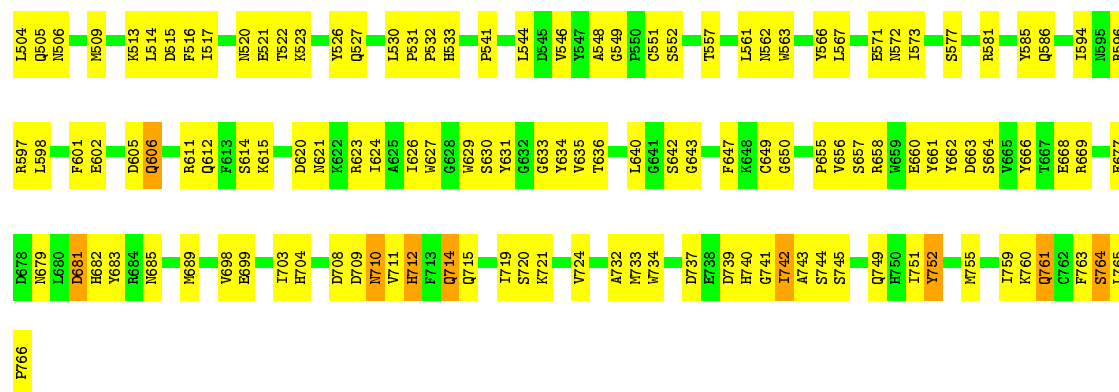




- Molecule 1: Dipeptidyl peptidase 4 (EC 3.4.14.5) (Dipeptidyl peptidase IV) (DPP IV) (T-cell activation antigen CD26) (TP103) (Adenosine deaminase complexing protein 2) (ADABP) (Dipeptidyl peptidase 4 soluble form) (Dipeptidyl peptidase IV soluble form)

Chain D: 47% 48% 5%







## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.18 Å   106.11 Å   132.05 Å 76.30°   78.62°   80.11°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	86.7 (20.00-3.10)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
13Z

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.56	0/6137	0.76	0/8346
1	B	0.56	0/6137	0.75	2/8346 (0.0%)
1	C	0.56	0/6137	0.73	2/8346 (0.0%)
1	D	0.56	0/6137	0.75	0/8346
All	All	0.56	0/24548	0.75	4/33384 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	214	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	415	LEU	N-CA-C	-5.60	95.89	111.00
1	C	388	GLN	N-CA-C	-5.33	96.60	111.00
1	B	388	GLN	N-CA-C	-5.11	97.20	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	TYR	Sidechain
1	A	700	TYR	Sidechain
1	B	128	TYR	Sidechain
1	C	83	TYR	Sidechain
1	D	752	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5965	0	5686	385	0
1	B	5965	0	5686	389	0
1	C	5965	0	5686	364	0
1	D	5965	0	5686	383	0
2	A	26	0	28	2	0
2	B	26	0	28	2	0
2	C	26	0	28	1	0
2	D	26	0	28	3	0
3	A	81	0	0	2	0
3	B	72	0	0	5	0
3	C	66	0	0	2	0
3	D	92	0	0	9	0
All	All	24275	0	22856	1490	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1490) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:TYR:HE2	1:D:184:ARG:HG2	1.07	1.12
1:D:173:TYR:CE2	1:D:184:ARG:HG2	1.89	1.06
1:A:253:ARG:HH21	1:B:253:ARG:NH1	1.55	1.05
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.41	1.03
1:A:154:TRP:CZ3	1:A:214:LEU:HD21	1.95	1.02
1:A:429:ARG:HG2	1:A:429:ARG:HH11	1.31	0.95
1:D:180:LEU:HB2	1:D:181:PRO:HD2	1.49	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ARG:HB2	1:C:687:THR:HG22	1.49	0.94
1:D:481:THR:HG1	1:D:483:HIS:HE2	1.07	0.93
1:D:143:ILE:HG23	1:D:179:ASN:OD1	1.67	0.93
1:A:286:GLN:HE21	1:A:288:THR:HG23	1.34	0.92
1:B:54:ARG:H	1:B:54:ARG:CD	1.83	0.92
1:A:154:TRP:HZ3	1:A:214:LEU:HD21	1.30	0.91
1:D:75:ASN:HD22	1:D:92:ASN:ND2	1.68	0.90
1:A:65:ASP:OD1	1:A:464:GLU:N	2.04	0.90
1:A:693:GLU:HG3	1:A:696:LYS:NZ	1.86	0.90
1:C:701:LEU:HD13	1:C:731:GLN:HB2	1.55	0.89
1:B:518:ILE:O	1:B:519:LEU:HD23	1.74	0.88
1:D:134:ILE:HD11	1:D:157:TRP:CH2	2.09	0.87
1:A:253:ARG:HH21	1:B:253:ARG:HH11	1.16	0.87
1:C:98:PHE:HE2	1:C:100:HIS:HB2	1.39	0.86
1:C:621:ASN:HD22	1:C:622:LYS:H	1.22	0.86
1:A:295:ILE:HD11	1:A:317:ARG:HH21	1.38	0.86
1:A:382:ARG:H	1:A:403:GLU:HG2	1.39	0.85
1:C:621:ASN:ND2	1:C:622:LYS:HG3	1.92	0.84
1:D:114:ILE:HG22	1:D:137:LEU:HD21	1.59	0.84
1:C:54:ARG:HH11	1:C:54:ARG:HG2	1.44	0.83
1:C:354:VAL:CG1	1:C:359:PRO:HG3	2.08	0.82
1:D:293:MET:HE2	1:D:317:ARG:HG3	1.60	0.82
1:D:621:ASN:HA	1:D:624:ILE:HD11	1.62	0.82
1:B:84:GLY:HA3	1:B:492:ARG:NH1	1.95	0.81
1:B:109:PRO:HG2	1:B:158:SER:O	1.81	0.81
1:B:658:ARG:HB2	1:B:687:THR:HG22	1.62	0.81
1:B:433:LYS:HD3	1:B:445:LEU:HD11	1.62	0.80
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.63	0.80
1:A:230:ASP:OD1	1:A:264:PRO:HB3	1.82	0.80
1:C:369:ASN:C	1:C:389:ILE:HG23	2.01	0.80
1:B:765:LEU:HB2	1:B:766:PRO:C	2.02	0.80
1:A:718:GLN:NE2	1:B:244:GLU:HA	1.96	0.80
1:A:65:ASP:OD2	1:A:466:LYS:HB2	1.83	0.79
1:D:134:ILE:HD11	1:D:157:TRP:HH2	1.47	0.79
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.18	0.79
1:D:549:GLY:O	1:D:552:SER:HB3	1.83	0.79
1:B:139:LYS:O	1:B:141:GLN:HG3	1.82	0.78
1:C:622:LYS:O	1:C:623:ARG:HG3	1.83	0.78
1:B:75:ASN:O	1:B:77:LEU:HD13	1.83	0.78
1:B:660:GLU:OE2	1:B:684:ARG:NH2	2.18	0.77
1:D:336:ARG:HG3	1:D:337:TRP:H	1.49	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ILE:HD11	1:A:317:ARG:NH2	1.99	0.77
1:D:272:ASN:C	1:D:272:ASN:HD22	1.88	0.77
1:C:119:ASN:O	1:C:130:ALA:HA	1.84	0.77
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.20	0.77
1:D:143:ILE:HG13	3:D:822:HOH:O	1.84	0.77
1:C:722:ALA:O	1:C:726:VAL:HG22	1.85	0.76
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.21	0.76
1:A:405:ILE:HG13	1:A:429:ARG:HD3	1.67	0.76
1:D:387:PHE:CE1	1:D:394:CYS:HB3	2.21	0.76
1:C:651:ILE:CD1	1:C:755:MET:HE2	2.15	0.76
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.68	0.76
1:A:218:PRO:HB2	1:A:308:GLN:NE2	2.01	0.76
1:C:651:ILE:HD13	1:C:755:MET:HE2	1.66	0.76
1:C:658:ARG:NH2	1:C:684:ARG:HD3	2.01	0.75
1:D:134:ILE:HD13	1:D:178:PRO:HB3	1.68	0.75
1:D:110:ASP:O	1:D:112:GLN:N	2.19	0.75
1:D:765:LEU:HB2	1:D:766:PRO:O	1.87	0.75
1:B:54:ARG:H	1:B:54:ARG:HD3	1.50	0.75
1:C:631:TYR:O	1:C:634:TYR:HB3	1.87	0.75
1:B:71:LYS:HE3	1:B:105:TYR:HE1	1.51	0.74
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.20	0.74
1:C:542:LEU:HD23	1:C:542:LEU:C	2.06	0.74
1:D:47:ASP:OD2	1:D:52:THR:HG21	1.87	0.74
1:B:134:ILE:HB	1:B:143:ILE:HD12	1.69	0.74
1:A:214:LEU:HD23	1:A:214:LEU:O	1.88	0.74
1:D:310:ARG:HG3	1:D:329:ASP:OD1	1.87	0.73
1:A:50:LYS:O	1:A:51:ASN:HB2	1.86	0.73
1:D:598:LEU:HD22	1:D:631:TYR:OH	1.87	0.73
1:D:236:ILE:HG12	1:D:712:HIS:CE1	2.23	0.73
1:D:571:GLU:CD	1:D:760:LYS:HD3	2.08	0.73
1:A:159:PRO:HG3	1:A:217:SER:O	1.87	0.73
1:A:55:LEU:HD12	1:A:500:LEU:HD22	1.69	0.73
1:D:626:ILE:HG23	1:D:636:THR:HG23	1.69	0.73
1:C:621:ASN:HD22	1:C:622:LYS:N	1.85	0.73
1:D:369:ASN:O	1:D:389:ILE:HG23	1.89	0.73
1:A:397:ILE:HD12	1:A:434:ILE:HG21	1.70	0.73
1:C:121:VAL:O	1:C:128:TYR:HB2	1.89	0.73
1:C:354:VAL:HG12	1:C:359:PRO:HG3	1.71	0.73
1:D:133:ASP:CG	1:D:147:ARG:HH21	1.91	0.73
1:D:235:LEU:HD23	1:D:255:PRO:HA	1.71	0.73
1:B:329:ASP:OD1	1:B:343:ARG:NH1	2.21	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ASN:O	1:B:389:ILE:HG23	1.88	0.73
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.69	0.72
1:B:123:GLN:HB3	1:B:127:SER:OG	1.89	0.72
1:B:432:TYR:CE2	1:B:444:CYS:HB2	2.24	0.72
1:C:114:ILE:HG22	1:C:137:LEU:HD21	1.71	0.72
1:C:79:PHE:CE1	1:C:86:SER:HB3	2.25	0.72
1:A:150:ASN:O	1:A:151:ASN:HB2	1.90	0.72
1:D:167:VAL:HG21	1:D:198:ILE:HG23	1.70	0.72
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.25	0.71
1:D:135:TYR:OH	1:D:140:ARG:HG2	1.90	0.71
1:D:272:ASN:HD22	1:D:273:THR:N	1.87	0.71
1:D:293:MET:CE	1:D:317:ARG:HG3	2.20	0.71
1:B:487:ASN:HD22	1:B:489:LYS:H	1.38	0.71
1:D:158:SER:CB	1:D:163:LYS:HB2	2.19	0.71
1:A:376:SER:HA	1:A:381:TYR:O	1.89	0.71
1:C:382:ARG:HH11	1:C:382:ARG:HG2	1.55	0.71
1:A:258:LYS:HZ3	1:A:712:HIS:CD2	2.09	0.71
1:A:415:LEU:HB2	1:A:436:LEU:HD21	1.71	0.71
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.71	0.71
1:C:146:GLU:OE1	1:C:181:PRO:HB3	1.90	0.71
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.71	0.71
1:A:134:ILE:HD11	1:A:164:LEU:HD11	1.72	0.71
1:C:516:PHE:CD2	1:C:523:LYS:HB2	2.26	0.71
1:D:517:ILE:HD12	1:D:612:GLN:HG3	1.73	0.71
1:D:272:ASN:ND2	1:D:274:ASP:H	1.88	0.71
1:C:137:LEU:O	1:C:140:ARG:HD2	1.90	0.71
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.89	0.70
1:C:420:ASN:HD22	1:C:426:PRO:HA	1.56	0.70
1:C:458:SER:HB3	1:C:471:ARG:HB3	1.71	0.70
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.73	0.70
1:C:596:ARG:O	1:C:597:ARG:HD2	1.91	0.70
1:B:603:VAL:HG22	1:B:635:VAL:HG13	1.73	0.70
1:B:519:LEU:O	1:B:522:THR:N	2.24	0.70
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.72	0.70
1:C:55:LEU:CD1	1:C:561:LEU:HD12	2.21	0.70
1:C:65:ASP:OD1	1:C:464:GLU:N	2.24	0.70
1:A:429:ARG:HG2	1:A:429:ARG:NH1	2.06	0.70
1:D:134:ILE:CG2	1:D:143:ILE:HD12	2.21	0.70
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.27	0.69
1:B:93:SER:HA	1:B:96:ASP:OD1	1.92	0.69
1:C:139:LYS:O	1:C:139:LYS:HG3	1.91	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ASN:OD1	1:D:139:LYS:N	2.25	0.69
1:A:693:GLU:HG3	1:A:696:LYS:HZ1	1.57	0.69
1:C:258:LYS:NZ	1:C:712:HIS:HD2	1.91	0.69
1:D:40:ARG:HB3	1:D:506:ASN:O	1.93	0.69
1:A:286:GLN:NE2	1:A:288:THR:HG23	2.05	0.69
1:C:658:ARG:HE	1:C:687:THR:HG21	1.56	0.69
1:A:258:LYS:NZ	1:A:712:HIS:CD2	2.61	0.69
1:A:477:LEU:HD13	1:A:500:LEU:HD23	1.74	0.69
1:B:674:PRO:O	1:B:680:LEU:HD13	1.93	0.69
1:D:95:PHE:CE1	1:D:116:LEU:HD11	2.28	0.69
1:A:248:TYR:CE2	1:B:258:LYS:HD2	2.28	0.69
1:B:680:LEU:HD11	1:B:684:ARG:CZ	2.23	0.69
1:C:633:GLY:HA3	1:C:655:PRO:HB3	1.73	0.69
1:B:487:ASN:ND2	1:B:489:LYS:H	1.90	0.68
1:B:602:GLU:OE2	1:B:602:GLU:N	2.26	0.68
1:C:184:ARG:NH1	1:C:187:TRP:HA	2.09	0.68
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.23	0.68
1:A:127:SER:HB3	1:A:211:TYR:CG	2.28	0.68
1:A:235:LEU:HD23	1:A:255:PRO:HA	1.75	0.68
1:C:365:THR:O	1:C:368:GLY:N	2.26	0.68
1:C:369:ASN:O	1:C:389:ILE:HG23	1.93	0.68
1:C:654:ALA:HA	1:C:704:HIS:ND1	2.09	0.68
1:D:235:LEU:HD23	1:D:255:PRO:CA	2.24	0.68
1:B:388:GLN:HG2	1:B:391:LYS:HE3	1.76	0.68
1:A:459:VAL:HG22	1:A:460:SER:H	1.58	0.68
1:C:258:LYS:HD2	1:D:248:TYR:CE2	2.28	0.68
1:B:667:THR:O	1:B:671:MET:HB2	1.93	0.68
1:D:195:TYR:O	1:D:227:GLN:HA	1.94	0.68
1:D:62:TRP:CE3	1:D:462:SER:HB3	2.29	0.68
1:A:621:ASN:HA	1:A:624:ILE:HD11	1.77	0.67
1:B:702:LEU:HD21	1:B:716:SER:HB3	1.76	0.67
1:B:745:SER:O	1:B:749:GLN:HG3	1.94	0.67
1:C:458:SER:CB	1:C:471:ARG:HD3	2.23	0.67
1:C:542:LEU:HD23	1:C:543:LEU:N	2.08	0.67
1:D:134:ILE:HG23	1:D:143:ILE:HD12	1.76	0.67
1:A:244:GLU:HA	1:B:718:GLN:NE2	2.10	0.67
1:B:470:LEU:HD12	1:B:483:HIS:NE2	2.09	0.67
1:A:263:ASN:ND2	1:A:318:ARG:CZ	2.58	0.67
1:B:516:PHE:HE2	1:B:518:ILE:HD11	1.59	0.67
1:B:534:PHE:HE1	1:B:574:ILE:HD11	1.58	0.67
1:C:216:TRP:CZ3	1:C:273:THR:HG21	2.30	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:720:SER:O	1:C:724:VAL:HG23	1.95	0.67
1:C:117:GLU:HB2	1:C:132:TYR:CE2	2.30	0.67
1:C:244:GLU:HG3	1:D:689:MET:HE3	1.76	0.67
1:D:108:SER:HB3	1:D:157:TRP:CE2	2.30	0.67
1:D:319:ILE:O	1:D:321:ASN:N	2.28	0.67
1:A:502:LYS:O	1:A:505:GLN:HG2	1.95	0.67
1:B:113:PHE:CE2	1:B:178:PRO:HG2	2.30	0.67
1:B:635:VAL:O	1:B:639:VAL:HG23	1.95	0.67
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.77	0.67
1:C:507:VAL:HG13	1:C:509:MET:HG2	1.76	0.67
1:D:139:LYS:HG2	1:D:141:GLN:HB2	1.77	0.67
1:D:214:LEU:HD12	1:D:223:LEU:HD11	1.77	0.66
1:C:93:SER:O	1:C:96:ASP:HB2	1.95	0.66
1:D:763:PHE:HB2	1:D:765:LEU:HD21	1.77	0.66
1:B:483:HIS:HD1	1:B:490:GLY:HA2	1.60	0.66
1:C:74:ASN:O	1:C:92:ASN:HA	1.95	0.66
1:D:745:SER:O	1:D:749:GLN:HG3	1.94	0.66
1:D:125:ARG:NH2	1:D:205:GLU:OE2	2.27	0.66
1:B:242:SER:CB	1:B:246:LEU:HD23	2.25	0.66
1:C:235:LEU:HD23	1:C:255:PRO:HA	1.77	0.66
1:C:761:GLN:NE2	1:C:762:CYS:HA	2.11	0.66
1:D:492:ARG:HB3	1:D:492:ARG:NH1	2.11	0.66
1:C:420:ASN:ND2	1:C:426:PRO:HA	2.11	0.66
1:A:175:LYS:CG	1:A:182:SER:HB3	2.23	0.66
1:B:518:ILE:CD1	1:B:523:LYS:HB3	2.25	0.66
1:A:263:ASN:HD22	1:A:318:ARG:CZ	2.09	0.65
1:C:72:GLN:O	1:C:75:ASN:HB2	1.97	0.65
1:A:113:PHE:CZ	1:A:178:PRO:HG2	2.31	0.65
1:A:156:THR:HG23	1:A:165:ALA:HB3	1.78	0.65
1:A:240:PHE:HB3	1:A:250:LYS:HG3	1.77	0.65
1:C:702:LEU:HD11	1:C:716:SER:OG	1.95	0.65
1:B:242:SER:HB3	1:B:246:LEU:HD23	1.79	0.65
1:B:514:LEU:HD22	1:B:557:THR:HG22	1.78	0.65
1:B:58:TYR:CD2	1:B:494:LEU:HB3	2.31	0.65
1:B:644:SER:O	1:B:646:VAL:HG23	1.97	0.65
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.32	0.65
1:A:64:SER:O	1:A:463:LYS:HG2	1.97	0.65
1:C:65:ASP:OD2	1:C:464:GLU:HB2	1.96	0.65
1:D:365:THR:O	1:D:368:GLY:N	2.24	0.65
1:C:513:LYS:O	1:C:527:GLN:HA	1.96	0.65
1:C:458:SER:HB3	1:C:471:ARG:HD3	1.77	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:VAL:HG22	1:C:508:GLN:N	2.12	0.65
1:C:125:ARG:HG2	1:C:126:HIS:CE1	2.32	0.65
1:A:511:SER:OG	1:A:530:LEU:HB2	1.96	0.64
1:C:114:ILE:CG2	1:C:137:LEU:HD21	2.26	0.64
1:D:397:ILE:HD12	1:D:434:ILE:HD13	1.77	0.64
1:C:535:ASP:OD1	1:C:538:LYS:HE2	1.96	0.64
1:D:57:LEU:HD12	1:D:57:LEU:H	1.62	0.64
1:A:218:PRO:HB2	1:A:308:GLN:CD	2.18	0.64
1:A:381:TYR:CE2	1:A:401:THR:HA	2.32	0.64
1:C:581:ARG:HB2	1:C:605:ASP:OD2	1.97	0.64
1:A:459:VAL:HG22	1:A:460:SER:N	2.11	0.64
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.31	0.64
1:C:244:GLU:HG3	1:D:689:MET:CE	2.27	0.64
1:D:146:GLU:HB2	1:D:179:ASN:O	1.96	0.64
1:D:571:GLU:O	1:D:573:ILE:HG13	1.97	0.64
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.95	0.64
1:C:745:SER:O	1:C:749:GLN:HG3	1.98	0.64
1:C:75:ASN:HD21	1:C:92:ASN:ND2	1.95	0.64
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.79	0.64
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.78	0.64
1:C:127:SER:HB3	1:C:211:TYR:CD1	2.33	0.64
1:D:159:PRO:HG3	1:D:217:SER:O	1.97	0.64
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.27	0.64
1:C:258:LYS:HZ1	1:C:712:HIS:HD2	1.45	0.64
1:D:515:ASP:OD2	1:D:516:PHE:N	2.30	0.64
1:A:260:GLY:HA3	1:A:674:PRO:HG3	1.79	0.63
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.80	0.63
1:D:492:ARG:HB3	1:D:492:ARG:HH11	1.63	0.63
1:B:446:SER:O	1:B:449:LEU:HG	1.98	0.63
1:A:58:TYR:CE2	1:A:494:LEU:HD13	2.33	0.63
1:A:68:TYR:CE1	1:A:79:PHE:HB2	2.34	0.63
1:C:90:LEU:HD21	1:C:95:PHE:HE2	1.63	0.63
1:B:130:ALA:HB3	1:B:132:TYR:CE1	2.33	0.63
1:C:336:ARG:HG3	1:C:336:ARG:HH11	1.64	0.63
1:D:548:ALA:HB3	1:D:635:VAL:HG21	1.81	0.63
1:A:158:SER:HB3	1:A:163:LYS:HB2	1.79	0.63
1:B:426:PRO:HG3	1:B:525:TRP:CD1	2.33	0.63
1:C:127:SER:HB3	1:C:211:TYR:CG	2.34	0.63
1:C:702:LEU:HD21	1:C:716:SER:HB3	1.81	0.63
1:D:173:TYR:HE2	1:D:184:ARG:CG	1.98	0.63
1:D:217:SER:HB2	1:D:222:PHE:HB2	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:O	1:A:193:ILE:HD13	1.99	0.63
1:B:71:LYS:HE3	1:B:105:TYR:CE1	2.31	0.63
1:C:383:HIS:HB3	1:C:398:THR:OG1	1.97	0.63
1:C:54:ARG:NH1	1:C:54:ARG:HG2	2.11	0.63
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.34	0.62
1:B:290:PRO:HD3	1:B:326:ASP:OD2	2.00	0.62
1:C:170:ASN:HD22	1:C:170:ASN:N	1.97	0.62
1:C:354:VAL:HG11	1:C:359:PRO:HG3	1.80	0.62
1:D:370:SER:HB2	1:D:387:PHE:O	2.00	0.62
1:B:513:LYS:NZ	1:B:515:ASP:HB2	2.14	0.62
1:B:54:ARG:N	1:B:54:ARG:CD	2.60	0.62
1:C:135:TYR:CD1	1:C:141:GLN:O	2.52	0.62
1:D:649:CYS:HB3	1:D:699:GLU:HB2	1.82	0.62
1:A:62:TRP:CG	1:A:462:SER:HA	2.34	0.62
1:D:75:ASN:HD22	1:D:92:ASN:HD22	1.45	0.62
1:B:516:PHE:CE2	1:B:523:LYS:HE2	2.34	0.62
1:D:596:ARG:O	1:D:597:ARG:HD2	2.00	0.62
1:A:168:TRP:O	1:A:169:ASN:HB2	1.99	0.62
1:A:673:LEU:HB2	1:A:678:ASP:OD2	2.00	0.62
1:C:376:SER:HA	1:C:382:ARG:HA	1.82	0.62
1:A:461:PHE:CE2	1:A:468:TYR:HB3	2.35	0.62
1:C:118:TYR:O	1:C:130:ALA:HB1	1.99	0.62
1:D:75:ASN:ND2	1:D:92:ASN:ND2	2.44	0.62
1:A:693:GLU:HG3	1:A:696:LYS:HZ2	1.62	0.61
1:D:40:ARG:HH11	1:D:40:ARG:HG3	1.65	0.61
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.47	0.61
1:B:145:GLU:O	1:B:146:GLU:C	2.38	0.61
1:B:75:ASN:HD22	1:B:92:ASN:ND2	1.98	0.61
1:C:492:ARG:HH11	1:C:492:ARG:HB3	1.65	0.61
1:D:336:ARG:HG3	1:D:337:TRP:N	2.14	0.61
1:A:675:THR:HB	1:A:676:PRO:HD2	1.81	0.61
1:C:550:PRO:HD3	1:C:631:TYR:CE2	2.35	0.61
1:C:73:GLU:O	1:C:75:ASN:N	2.34	0.61
1:B:486:VAL:HG13	1:B:487:ASN:N	2.15	0.61
1:A:453:ARG:HG2	1:A:454:CYS:SG	2.41	0.61
1:A:81:ALA:O	1:A:491:LEU:HD13	2.01	0.61
1:B:268:PHE:CE2	1:B:313:LEU:HD21	2.35	0.61
1:D:133:ASP:OD2	1:D:147:ARG:NH2	2.32	0.61
1:D:433:LYS:HB2	1:D:445:LEU:HD11	1.81	0.61
1:B:528:MET:HG2	1:B:576:ALA:HB2	1.82	0.61
1:D:387:PHE:CD1	1:D:394:CYS:HB3	2.35	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HD11	1:A:105:TYR:CE1	2.36	0.61
1:B:92:ASN:OD1	1:B:93:SER:N	2.33	0.61
1:A:71:LYS:HG3	1:A:76:ILE:HG12	1.83	0.61
1:B:658:ARG:HH22	1:B:684:ARG:HD3	1.66	0.61
1:C:455:GLN:HB2	1:C:475:PRO:HD3	1.82	0.61
1:C:658:ARG:HH22	1:C:684:ARG:HD3	1.66	0.61
1:B:414:TYR:CD2	1:B:433:LYS:HG2	2.36	0.61
1:C:541:PRO:HB2	1:C:763:PHE:CE2	2.36	0.61
1:D:136:ASP:OD1	1:D:138:ASN:HB3	2.00	0.61
1:D:167:VAL:HA	1:D:171:ASP:O	2.01	0.61
1:A:730:PHE:HD1	1:A:731:GLN:O	1.84	0.61
1:A:253:ARG:NH2	1:B:253:ARG:HH11	1.94	0.61
1:B:741:GLY:O	1:B:742:ILE:C	2.39	0.61
1:D:235:LEU:HD21	1:D:255:PRO:HG3	1.82	0.61
1:D:414:TYR:CE2	1:D:433:LYS:HE3	2.36	0.61
1:C:218:PRO:HB2	1:C:308:GLN:NE2	2.16	0.60
1:A:138:ASN:C	1:A:140:ARG:H	2.03	0.60
1:B:75:ASN:ND2	1:B:92:ASN:ND2	2.49	0.60
1:B:237:GLU:OE2	1:B:253:ARG:HD3	2.01	0.60
1:A:403:GLU:OE2	1:A:587:GLY:N	2.34	0.60
1:C:726:VAL:HG23	1:C:728:VAL:CG1	2.32	0.60
1:D:241:TYR:O	1:D:246:LEU:HD23	2.01	0.60
1:D:751:ILE:HG23	1:D:752:TYR:N	2.16	0.60
1:A:438:ASP:O	1:A:440:THR:N	2.35	0.60
1:A:470:LEU:HD12	1:A:483:HIS:NE2	2.16	0.60
1:A:95:PHE:CB	1:A:98:PHE:HB2	2.31	0.60
1:B:429:ARG:HG3	1:B:456:TYR:CZ	2.37	0.60
1:C:134:ILE:HD13	1:C:178:PRO:HB3	1.83	0.60
1:D:208:PHE:HE1	1:D:300:LEU:O	1.84	0.60
1:B:150:ASN:O	1:B:151:ASN:HB2	2.02	0.60
1:B:152:THR:HG23	1:B:167:VAL:O	2.01	0.60
1:B:106:SER:HG	1:B:157:TRP:HE1	1.50	0.60
1:C:105:TYR:O	1:C:106:SER:HB2	2.02	0.60
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.31	0.60
1:D:134:ILE:HG21	1:D:178:PRO:HB2	1.81	0.60
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.83	0.60
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.83	0.60
1:C:258:LYS:NZ	1:C:712:HIS:CD2	2.70	0.60
1:C:82:GLU:HG2	1:C:83:TYR:CZ	2.37	0.60
1:D:765:LEU:HB2	1:D:766:PRO:C	2.22	0.60
1:A:75:ASN:N	1:A:92:ASN:HB3	2.17	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:CZ	1:B:258:LYS:HD2	2.36	0.60
1:B:122:LYS:HG2	1:B:123:GLN:N	2.16	0.60
1:B:199:THR:HA	1:B:228:PHE:CE2	2.37	0.60
1:C:73:GLU:C	1:C:75:ASN:H	2.06	0.59
1:D:110:ASP:C	1:D:112:GLN:H	2.05	0.59
1:A:432:TYR:CE2	1:A:444:CYS:HB2	2.38	0.59
1:A:42:THR:HB	1:A:569:SER:OG	2.03	0.59
1:A:631:TYR:O	1:A:634:TYR:HB3	2.01	0.59
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.37	0.59
1:B:159:PRO:O	1:B:160:VAL:HG23	2.02	0.59
1:D:272:ASN:ND2	1:D:272:ASN:C	2.55	0.59
1:D:268:PHE:CZ	1:D:313:LEU:HD21	2.37	0.59
1:A:148:ILE:HD12	1:A:148:ILE:H	1.67	0.59
1:A:227:GLN:O	1:A:266:VAL:HA	2.01	0.59
1:A:611:ARG:O	1:A:614:SER:HB3	2.03	0.59
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.99	0.59
1:B:52:THR:O	1:B:54:ARG:NH1	2.31	0.59
1:B:206:GLU:OE1	2:B:767:13Z:H15	2.02	0.59
1:C:580:GLY:O	1:C:583:SER:OG	2.20	0.59
1:C:658:ARG:HE	1:C:687:THR:CG2	2.15	0.59
1:C:720:SER:HB2	1:C:730:PHE:HZ	1.67	0.59
1:C:49:LEU:CD2	1:C:749:GLN:HA	2.31	0.59
1:D:235:LEU:CD2	1:D:255:PRO:HG3	2.32	0.59
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.38	0.59
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.82	0.59
1:D:708:ASP:OD2	1:D:740:HIS:HA	2.02	0.59
1:A:286:GLN:HE21	1:A:288:THR:CG2	2.11	0.59
1:D:602:GLU:OE2	1:D:602:GLU:N	2.32	0.59
1:D:614:SER:HB2	1:D:621:ASN:OD1	2.03	0.59
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.36	0.59
1:A:293:MET:HE3	1:A:315:TRP:O	2.01	0.59
1:A:57:LEU:N	1:A:57:LEU:HD12	2.17	0.59
1:B:555:ALA:HB3	1:B:579:ASP:OD2	2.02	0.59
1:D:487:ASN:H	1:D:487:ASN:HD22	1.49	0.59
1:A:446:SER:HB2	1:A:457:TYR:CE2	2.38	0.59
1:A:644:SER:HB2	1:A:646:VAL:HG23	1.85	0.59
1:D:316:LEU:HD21	1:D:320:GLN:HG2	1.85	0.59
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.03	0.59
1:A:726:VAL:HG23	1:A:728:VAL:HG12	1.83	0.59
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.85	0.59
1:B:611:ARG:O	1:B:615:LYS:HG2	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ARG:HH12	1:C:682:HIS:HB2	1.68	0.59
1:C:621:ASN:ND2	1:C:622:LYS:H	1.98	0.59
1:C:634:TYR:HD1	1:C:656:VAL:O	1.85	0.59
1:D:370:SER:HG	1:D:386:TYR:HE1	1.49	0.59
1:B:765:LEU:H	1:B:765:LEU:HD22	1.68	0.59
1:D:664:SER:HB2	1:D:668:GLU:OE2	2.02	0.59
1:B:355:GLY:HA2	1:B:382:ARG:HH12	1.68	0.59
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.03	0.58
1:C:174:VAL:O	1:C:183:TYR:HD2	1.84	0.58
1:D:743:ALA:O	1:D:744:SER:C	2.39	0.58
1:C:658:ARG:HB2	1:C:687:THR:CG2	2.29	0.58
1:D:118:TYR:O	1:D:130:ALA:HB1	2.02	0.58
1:C:58:TYR:HD2	1:C:58:TYR:O	1.86	0.58
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.85	0.58
1:D:159:PRO:HD3	1:D:216:TRP:HB3	1.85	0.58
1:D:486:VAL:HG13	1:D:487:ASN:N	2.19	0.58
1:A:369:ASN:C	1:A:389:ILE:HG23	2.23	0.58
1:A:472:CYS:O	1:A:478:PRO:HA	2.04	0.58
1:A:524:PHE:HD2	1:A:580:GLY:HA2	1.69	0.58
1:B:208:PHE:O	1:B:209:SER:HB2	2.03	0.58
1:D:513:LYS:O	1:D:527:GLN:HA	2.02	0.58
1:D:422:TYR:CE2	1:D:423:LYS:HE2	2.39	0.58
1:D:633:GLY:C	1:D:655:PRO:HB3	2.24	0.58
1:A:468:TYR:CE2	1:A:483:HIS:HB2	2.38	0.58
1:B:135:TYR:CE2	1:B:140:ARG:HA	2.37	0.58
1:D:113:PHE:CD2	1:D:113:PHE:N	2.71	0.58
1:B:122:LYS:CG	1:B:123:GLN:N	2.67	0.58
1:D:114:ILE:HG22	1:D:137:LEU:CD2	2.31	0.58
1:D:184:ARG:NH1	1:D:187:TRP:HA	2.18	0.58
1:C:325:MET:HE3	1:C:371:PHE:CE2	2.38	0.58
1:D:191:GLU:O	1:D:192:ASP:HB2	2.03	0.58
1:D:74:ASN:C	1:D:92:ASN:HB3	2.24	0.58
1:A:260:GLY:HA3	1:A:674:PRO:CG	2.34	0.58
1:B:54:ARG:H	1:B:54:ARG:HD2	1.65	0.58
1:C:516:PHE:HD2	1:C:523:LYS:HB2	1.66	0.58
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.85	0.58
1:A:75:ASN:OD1	1:A:91:GLU:HA	2.03	0.57
1:B:125:ARG:NH2	1:B:205:GLU:OE2	2.37	0.57
1:B:544:LEU:HD21	1:B:606:GLN:HG3	1.84	0.57
1:C:621:ASN:HD21	1:C:622:LYS:HG3	1.68	0.57
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:SER:HB3	1:A:471:ARG:HD3	1.85	0.57
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.39	0.57
1:B:751:ILE:O	1:B:755:MET:HG3	2.04	0.57
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.39	0.57
1:C:644:SER:HB2	1:C:646:VAL:HG23	1.85	0.57
1:C:751:ILE:O	1:C:755:MET:HG3	2.03	0.57
1:D:455:GLN:NE2	1:D:475:PRO:HG3	2.19	0.57
1:D:765:LEU:N	1:D:765:LEU:HD22	2.20	0.57
1:A:415:LEU:HD23	1:A:415:LEU:C	2.25	0.57
1:B:113:PHE:CD1	1:B:136:ASP:HA	2.40	0.57
1:C:77:LEU:HD22	1:C:87:SER:O	2.05	0.57
1:D:314:GLN:NE2	1:D:362:PRO:HD3	2.20	0.57
1:B:443:THR:HG22	1:B:445:LEU:HD23	1.86	0.57
1:D:266:VAL:O	1:D:267:LYS:HG2	2.04	0.57
1:D:374:ILE:CD1	1:D:404:VAL:HG12	2.35	0.57
1:B:272:ASN:C	1:B:272:ASN:HD22	2.08	0.57
1:B:301:CYS:O	1:B:358:ARG:NH1	2.37	0.57
1:B:459:VAL:HG22	1:B:460:SER:N	2.18	0.57
1:C:236:ILE:HD12	1:C:237:GLU:H	1.67	0.57
1:C:56:LYS:HD3	1:C:495:GLU:OE1	2.05	0.57
1:C:63:ILE:HG21	1:C:69:LEU:HG	1.84	0.57
1:D:336:ARG:CG	1:D:337:TRP:N	2.68	0.57
1:A:524:PHE:CD2	1:A:580:GLY:HA2	2.40	0.57
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.86	0.57
1:C:387:PHE:CE1	1:C:394:CYS:HB3	2.39	0.57
1:C:621:ASN:HD22	1:C:621:ASN:N	2.01	0.57
1:D:180:LEU:HB2	1:D:181:PRO:CD	2.30	0.57
1:D:516:PHE:CD2	1:D:523:LYS:HB2	2.38	0.57
1:D:544:LEU:HD21	1:D:606:GLN:HG3	1.87	0.57
1:A:175:LYS:HG3	1:A:182:SER:CB	2.25	0.57
1:B:146:GLU:OE1	1:B:181:PRO:HB3	2.05	0.57
1:D:658:ARG:O	1:D:661:TYR:HB2	2.04	0.57
1:D:75:ASN:ND2	1:D:92:ASN:HD22	2.01	0.57
1:B:464:GLU:O	1:B:465:ALA:HB3	2.04	0.56
1:A:143:ILE:HD13	1:A:178:PRO:HB2	1.87	0.56
1:C:545:ASP:OD1	1:C:554:LYS:NZ	2.35	0.56
1:A:433:LYS:HD3	1:A:445:LEU:HD21	1.87	0.56
1:A:580:GLY:O	1:A:581:ARG:C	2.43	0.56
1:C:620:ASP:OD2	1:C:623:ARG:HD3	2.05	0.56
1:C:657:SER:HB3	1:C:719:ILE:HD11	1.86	0.56
1:A:163:LYS:NZ	1:A:273:THR:OG1	2.37	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:HG2	1:A:315:TRP:CB	2.36	0.56
1:C:41:LYS:HG3	1:C:507:VAL:HG23	1.87	0.56
1:C:397:ILE:HD12	1:C:434:ILE:HD13	1.88	0.56
1:D:124:TRP:HA	1:D:124:TRP:CE3	2.41	0.56
1:A:736:THR:HG22	1:B:721:LYS:HD3	1.86	0.56
1:B:61:ARG:NH1	1:B:105:TYR:CE2	2.73	0.56
1:B:242:SER:OG	1:B:243:ASP:N	2.38	0.56
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.87	0.56
1:B:57:LEU:HA	1:B:480:TYR:CZ	2.41	0.56
1:B:535:ASP:O	1:B:537:SER:N	2.38	0.56
1:B:54:ARG:N	1:B:54:ARG:HD3	2.20	0.56
1:B:63:ILE:HG21	1:B:69:LEU:HG	1.86	0.56
1:B:487:ASN:HD22	1:B:489:LYS:N	2.03	0.56
1:A:116:LEU:O	1:A:132:TYR:HA	2.06	0.56
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.05	0.56
1:B:119:ASN:O	1:B:121:VAL:HG23	2.06	0.56
1:D:236:ILE:HG23	1:D:254:VAL:HG13	1.88	0.56
1:C:459:VAL:HG22	1:C:460:SER:N	2.20	0.56
1:C:711:VAL:HG12	1:C:715:GLN:HG3	1.87	0.56
1:D:169:ASN:HD22	1:D:169:ASN:N	2.03	0.56
1:D:253:ARG:HB2	1:D:253:ARG:HH11	1.71	0.56
1:D:422:TYR:CE2	1:D:423:LYS:HG3	2.41	0.56
1:D:765:LEU:H	1:D:766:PRO:HA	1.70	0.56
1:A:388:GLN:HB3	1:A:391:LYS:HB2	1.87	0.56
1:A:724:VAL:HG22	1:B:750:HIS:CD2	2.41	0.56
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.24	0.56
1:D:310:ARG:HH11	1:D:310:ARG:HG3	1.71	0.56
1:D:376:SER:OG	1:D:380:GLY:HA2	2.05	0.56
1:A:242:SER:OG	1:A:243:ASP:N	2.39	0.56
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.41	0.56
1:C:621:ASN:ND2	1:C:622:LYS:N	2.54	0.56
1:A:422:TYR:CZ	1:A:423:LYS:HE3	2.41	0.55
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.41	0.55
1:D:114:ILE:CG2	1:D:137:LEU:HD21	2.34	0.55
1:A:148:ILE:HD12	1:A:148:ILE:N	2.21	0.55
1:A:184:ARG:HD3	1:A:186:THR:O	2.07	0.55
1:D:267:LYS:HD2	1:D:286:GLN:HE22	1.71	0.55
1:D:484:SER:HB3	1:D:487:ASN:HD21	1.71	0.55
1:A:325:MET:CE	1:A:362:PRO:HG3	2.35	0.55
1:B:518:ILE:HD13	1:B:523:LYS:HB3	1.87	0.55
1:C:611:ARG:HG2	1:C:615:LYS:NZ	2.20	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLU:OE1	1:D:181:PRO:HA	2.06	0.55
1:A:504:LEU:HA	1:A:507:VAL:HG13	1.88	0.55
1:C:55:LEU:HD11	1:C:561:LEU:HD12	1.87	0.55
1:D:67:GLU:OE1	1:D:78:VAL:HG21	2.06	0.55
1:A:263:ASN:HD22	1:A:318:ARG:NH1	2.03	0.55
1:D:124:TRP:HA	1:D:124:TRP:HE3	1.71	0.55
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.87	0.55
1:D:765:LEU:N	1:D:766:PRO:HA	2.21	0.55
1:A:280:THR:HG22	1:A:281:ASN:H	1.71	0.55
1:B:379:GLU:HG3	3:B:809:HOH:O	2.06	0.55
1:D:241:TYR:O	1:D:242:SER:HB3	2.07	0.55
1:B:168:TRP:O	1:B:169:ASN:HB2	2.07	0.55
1:B:258:LYS:NZ	1:B:712:HIS:CD2	2.75	0.55
1:C:377:ASN:OD1	1:C:379:GLU:N	2.39	0.55
1:C:486:VAL:HG13	1:C:487:ASN:H	1.71	0.55
1:C:258:LYS:HZ3	1:C:712:HIS:CD2	2.25	0.55
1:A:458:SER:CB	1:A:471:ARG:HD3	2.37	0.55
1:B:658:ARG:HD2	1:B:661:TYR:CZ	2.42	0.55
1:B:657:SER:HB2	1:B:689:MET:SD	2.47	0.55
1:C:542:LEU:CD2	1:C:542:LEU:C	2.73	0.55
1:D:40:ARG:HD2	1:D:506:ASN:HA	1.88	0.55
1:A:408:GLU:HG3	1:A:418:ILE:HG13	1.88	0.55
1:A:143:ILE:CD1	1:A:178:PRO:HB2	2.36	0.54
1:B:538:LYS:O	1:B:618:PHE:HA	2.05	0.54
1:C:507:VAL:HG22	1:C:508:GLN:H	1.73	0.54
1:C:75:ASN:ND2	1:C:92:ASN:CG	2.60	0.54
1:D:47:ASP:HA	1:D:52:THR:CG2	2.38	0.54
1:D:741:GLY:O	1:D:742:ILE:C	2.45	0.54
1:A:360:SER:O	1:A:373:LYS:NZ	2.37	0.54
1:B:115:LEU:HD21	1:B:132:TYR:CD2	2.41	0.54
1:C:372:TYR:OH	1:C:436:LEU:HD22	2.07	0.54
1:C:732:ALA:HB1	1:D:734:TRP:CZ3	2.42	0.54
1:D:174:VAL:HG23	1:D:185:ILE:CG1	2.38	0.54
1:A:142:LEU:O	1:A:144:THR:HG23	2.08	0.54
1:A:158:SER:HA	1:A:216:TRP:CE2	2.43	0.54
1:B:627:TRP:HA	1:B:651:ILE:O	2.08	0.54
1:B:75:ASN:HB3	1:B:92:ASN:N	2.22	0.54
1:C:420:ASN:HD22	1:C:426:PRO:CA	2.20	0.54
1:D:158:SER:OG	1:D:163:LYS:HB2	2.07	0.54
1:D:611:ARG:O	1:D:615:LYS:HG2	2.06	0.54
1:A:340:LEU:O	1:A:343:ARG:N	2.38	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:TYR:CE2	1:C:184:ARG:HG2	2.43	0.54
1:A:154:TRP:CH2	1:A:156:THR:HB	2.43	0.54
1:C:195:TYR:HB3	1:C:198:ILE:O	2.07	0.54
1:C:651:ILE:HD12	1:C:755:MET:HE2	1.89	0.54
1:A:108:SER:O	1:A:111:GLY:N	2.39	0.54
1:A:242:SER:O	1:A:243:ASP:O	2.26	0.54
1:B:218:PRO:HB2	1:B:308:GLN:HE22	1.72	0.54
1:C:167:VAL:HA	1:C:171:ASP:O	2.08	0.54
1:C:370:SER:HA	1:C:387:PHE:O	2.08	0.54
1:A:142:LEU:O	1:A:143:ILE:C	2.45	0.54
1:A:154:TRP:CZ3	1:A:214:LEU:CD2	2.82	0.54
1:A:56:LYS:HB2	1:A:497:ASN:OD1	2.06	0.54
1:B:136:ASP:O	1:B:138:ASN:N	2.40	0.54
1:B:134:ILE:CB	1:B:143:ILE:HD12	2.37	0.54
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.42	0.54
1:C:58:TYR:O	1:C:58:TYR:CD2	2.60	0.54
1:A:548:ALA:HB3	1:A:635:VAL:HG21	1.90	0.54
1:B:75:ASN:ND2	1:B:92:ASN:HD22	2.05	0.54
1:D:74:ASN:O	1:D:92:ASN:HB3	2.08	0.54
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.28	0.54
1:D:657:SER:HB2	1:D:689:MET:SD	2.48	0.54
1:A:627:TRP:HB2	1:A:651:ILE:HB	1.90	0.54
1:A:736:THR:CG2	1:B:721:LYS:HD3	2.37	0.54
1:D:384:ILE:HG23	1:D:407:ILE:HD11	1.90	0.54
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.43	0.54
1:B:75:ASN:HB3	1:B:92:ASN:H	1.73	0.53
1:C:357:PHE:O	1:C:669:ARG:NH1	2.41	0.53
1:C:651:ILE:HG21	1:C:755:MET:CE	2.39	0.53
1:B:272:ASN:ND2	1:B:274:ASP:H	2.07	0.53
1:C:491:LEU:O	1:C:492:ARG:HB3	2.08	0.53
1:D:346:ILE:CG2	1:D:347:GLU:N	2.71	0.53
1:A:634:TYR:HD1	1:A:656:VAL:O	1.90	0.53
1:B:631:TYR:O	1:B:634:TYR:HB3	2.09	0.53
1:C:520:ASN:O	1:C:521:GLU:HB2	2.07	0.53
1:A:397:ILE:CD1	1:A:434:ILE:HG21	2.37	0.53
1:C:195:TYR:O	1:C:227:GLN:HA	2.09	0.53
1:D:321:ASN:HA	1:D:354:VAL:HG23	1.91	0.53
1:D:65:ASP:OD2	1:D:466:LYS:HD2	2.08	0.53
1:D:760:LYS:HD2	1:D:766:PRO:O	2.08	0.53
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.09	0.53
1:B:74:ASN:HB3	1:B:92:ASN:HB2	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:PRO:O	1:C:680:LEU:HD13	2.09	0.53
1:D:629:TRP:O	1:D:630:SER:HB3	2.08	0.53
1:A:170:ASN:OD1	1:A:194:ILE:O	2.26	0.53
1:A:236:ILE:CG2	1:A:254:VAL:HG13	2.39	0.53
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.08	0.53
1:B:60:LEU:C	1:B:60:LEU:HD12	2.29	0.53
1:B:708:ASP:OD2	1:B:740:HIS:HA	2.09	0.53
1:C:621:ASN:N	1:C:621:ASN:ND2	2.55	0.53
1:A:370:SER:HA	1:A:387:PHE:O	2.09	0.53
1:C:661:TYR:HB2	1:C:715:GLN:NE2	2.24	0.53
1:D:81:ALA:O	1:D:491:LEU:HD13	2.09	0.53
1:D:482:LEU:HD13	1:D:494:LEU:HD11	1.91	0.53
1:A:515:ASP:OD1	1:A:516:PHE:N	2.38	0.53
1:A:724:VAL:HA	1:B:750:HIS:HD2	1.74	0.53
1:A:74:ASN:C	1:A:92:ASN:HB3	2.29	0.53
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.09	0.53
1:B:658:ARG:NH2	1:B:684:ARG:HD3	2.23	0.53
1:C:127:SER:O	1:C:128:TYR:HB3	2.08	0.53
1:C:316:LEU:HD12	1:C:323:SER:HB3	1.90	0.53
1:D:360:SER:O	1:D:373:LYS:NZ	2.38	0.53
1:A:545:ASP:OD1	1:A:554:LYS:NZ	2.42	0.53
1:C:266:VAL:HG22	1:C:267:LYS:N	2.23	0.53
1:C:334:SER:OG	1:C:336:ARG:HG2	2.09	0.53
1:D:129:THR:O	1:D:130:ALA:HB2	2.09	0.53
1:B:293:MET:CE	1:B:317:ARG:HG3	2.39	0.52
1:C:110:ASP:OD2	1:C:112:GLN:HB2	2.10	0.52
1:D:199:THR:HA	1:D:228:PHE:CE2	2.45	0.52
1:D:77:LEU:HD12	1:D:77:LEU:N	2.24	0.52
1:B:428:GLY:O	1:B:429:ARG:HG2	2.09	0.52
1:D:487:ASN:H	1:D:487:ASN:ND2	2.07	0.52
1:D:73:GLU:N	1:D:73:GLU:CD	2.62	0.52
1:A:235:LEU:HD23	1:A:255:PRO:CA	2.39	0.52
1:A:385:CYS:HB3	1:A:387:PHE:HE2	1.74	0.52
1:B:516:PHE:CE2	1:B:518:ILE:HD11	2.43	0.52
1:B:664:SER:O	1:B:668:GLU:HB2	2.09	0.52
1:B:763:PHE:HB2	1:B:765:LEU:HD21	1.90	0.52
1:C:73:GLU:C	1:C:75:ASN:N	2.63	0.52
1:A:354:VAL:CG1	1:A:359:PRO:HG3	2.39	0.52
1:A:49:LEU:HD13	1:A:749:GLN:HA	1.92	0.52
1:A:684:ARG:HG3	1:A:684:ARG:HH11	1.74	0.52
1:B:155:VAL:HG12	1:B:156:THR:N	2.24	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:HA	1:B:252:VAL:O	2.09	0.52
1:B:765:LEU:HD22	1:B:765:LEU:N	2.25	0.52
1:C:324:VAL:HG22	1:C:346:ILE:HG12	1.90	0.52
1:D:241:TYR:O	1:D:242:SER:CB	2.57	0.52
1:D:640:LEU:HD22	1:D:698:VAL:HG21	1.91	0.52
1:A:208:PHE:O	1:A:209:SER:C	2.48	0.52
1:A:39:THR:HG23	1:A:40:ARG:H	1.72	0.52
1:A:431:LEU:CD2	1:A:445:LEU:HD12	2.39	0.52
1:A:445:LEU:HD22	1:A:488:ASP:OD1	2.08	0.52
1:A:610:ALA:O	1:A:613:PHE:N	2.42	0.52
1:C:170:ASN:O	1:C:196:ASN:HB2	2.10	0.52
1:C:312:SER:O	1:C:313:LEU:HD12	2.09	0.52
1:C:300:LEU:HD13	1:C:315:TRP:CH2	2.44	0.52
1:A:333:SER:OG	1:A:334:SER:N	2.41	0.52
1:A:621:ASN:HD22	1:A:621:ASN:N	2.08	0.52
1:C:80:ASN:O	1:C:84:GLY:N	2.39	0.52
1:D:218:PRO:HB2	1:D:308:GLN:OE1	2.09	0.52
1:D:541:PRO:HG2	1:D:573:ILE:HA	1.91	0.52
1:A:517:ILE:O	1:A:517:ILE:HG13	2.09	0.52
1:A:520:ASN:O	1:A:521:GLU:HB2	2.09	0.52
1:B:459:VAL:CG2	1:B:460:SER:N	2.73	0.52
1:D:301:CYS:SG	1:D:359:PRO:HD2	2.50	0.52
1:C:191:GLU:O	1:C:193:ILE:HG12	2.09	0.52
1:D:98:PHE:CD2	1:D:100:HIS:HB2	2.44	0.52
1:A:486:VAL:HG13	1:A:487:ASN:N	2.25	0.52
1:C:224:ALA:HA	1:C:270:VAL:HA	1.91	0.52
1:C:60:LEU:HD12	1:C:60:LEU:C	2.30	0.52
1:D:703:ILE:HG23	1:D:733:MET:O	2.09	0.52
1:A:718:GLN:HE22	1:B:244:GLU:HA	1.72	0.52
1:B:429:ARG:HG3	1:B:456:TYR:CE1	2.45	0.52
1:B:48:TYR:CE1	1:B:562:ASN:HA	2.45	0.52
1:A:177:GLU:HB2	1:A:180:LEU:HG	1.91	0.51
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.45	0.51
1:C:382:ARG:NH1	1:C:382:ARG:HG2	2.23	0.51
1:C:589:LYS:HB3	3:C:782:HOH:O	2.10	0.51
1:C:733:MET:HG3	1:C:735:TYR:CE1	2.45	0.51
1:D:268:PHE:CE2	1:D:313:LEU:HD21	2.45	0.51
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.45	0.51
1:B:208:PHE:N	1:B:208:PHE:CD1	2.76	0.51
1:B:629:TRP:O	1:B:630:SER:HB3	2.10	0.51
1:C:266:VAL:CG2	1:C:267:LYS:N	2.72	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:ASP:C	1:C:537:SER:H	2.14	0.51
1:D:236:ILE:HG12	1:D:712:HIS:ND1	2.25	0.51
1:A:742:ILE:HG22	1:A:742:ILE:O	2.10	0.51
1:B:459:VAL:HG23	1:B:469:GLN:O	2.10	0.51
1:C:173:TYR:HA	1:C:183:TYR:O	2.10	0.51
1:A:177:GLU:HB2	1:A:180:LEU:CG	2.40	0.51
1:B:134:ILE:CG2	1:B:143:ILE:HD12	2.41	0.51
1:B:57:LEU:HA	1:B:480:TYR:CE1	2.45	0.51
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.92	0.51
1:D:174:VAL:HG23	1:D:185:ILE:HD11	1.93	0.51
1:B:108:SER:HB3	1:B:157:TRP:CE3	2.44	0.51
1:C:184:ARG:HB3	1:C:187:TRP:CZ2	2.46	0.51
1:C:336:ARG:CG	1:C:336:ARG:HH11	2.22	0.51
1:D:134:ILE:HD13	1:D:178:PRO:CB	2.38	0.51
1:D:343:ARG:HA	1:D:389:ILE:O	2.11	0.51
1:D:343:ARG:O	1:D:345:HIS:ND1	2.43	0.51
1:A:382:ARG:N	1:A:403:GLU:HG2	2.17	0.51
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.92	0.51
1:B:552:SER:O	1:B:583:SER:HB2	2.09	0.51
1:C:148:ILE:HD12	1:C:148:ILE:H	1.76	0.51
1:A:134:ILE:HD11	1:A:164:LEU:CD1	2.41	0.51
1:A:66:HIS:CD2	1:A:67:GLU:HG3	2.46	0.51
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.59	0.51
1:B:115:LEU:HD11	1:B:132:TYR:HB3	1.93	0.51
1:B:242:SER:HB2	1:B:246:LEU:HD23	1.93	0.51
1:C:256:TYR:CZ	1:C:663:ASP:HB3	2.46	0.51
1:C:596:ARG:C	1:C:597:ARG:HD2	2.31	0.51
1:D:163:LYS:NZ	1:D:273:THR:OG1	2.44	0.51
1:D:146:GLU:HG3	1:D:181:PRO:N	2.26	0.51
1:D:331:ASP:HB3	1:D:334:SER:OG	2.10	0.51
1:A:146:GLU:HB2	1:A:179:ASN:O	2.11	0.51
1:B:217:SER:O	1:B:220:GLY:N	2.37	0.51
1:C:180:LEU:HB3	1:C:181:PRO:HD2	1.91	0.51
1:D:272:ASN:HD21	1:D:274:ASP:H	1.59	0.51
1:D:60:LEU:C	1:D:60:LEU:HD12	2.31	0.51
1:A:139:LYS:HE2	1:D:333:SER:OG	2.11	0.51
1:B:534:PHE:CE1	1:B:574:ILE:HD11	2.43	0.51
1:B:673:LEU:O	1:B:678:ASP:HB3	2.11	0.51
1:C:236:ILE:HD12	1:C:237:GLU:N	2.25	0.51
1:C:651:ILE:HG21	1:C:755:MET:HE2	1.93	0.51
1:D:415:LEU:C	1:D:415:LEU:HD23	2.31	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ALA:HB2	1:A:461:PHE:CD1	2.46	0.50
1:B:360:SER:O	1:B:373:LYS:HE2	2.11	0.50
1:C:168:TRP:O	1:C:169:ASN:HB2	2.12	0.50
1:C:231:THR:HG22	1:C:232:GLU:HG3	1.93	0.50
1:C:508:GLN:O	1:C:532:PRO:HG2	2.11	0.50
1:C:80:ASN:HB3	1:C:85:ASN:OD1	2.11	0.50
1:D:341:VAL:O	1:D:344:GLN:HB2	2.11	0.50
1:A:530:LEU:HD13	1:A:534:PHE:CD2	2.46	0.50
1:B:105:TYR:HD2	1:B:107:ILE:HD12	1.75	0.50
1:A:249:PRO:HD3	1:B:714:GLN:NE2	2.26	0.50
1:C:736:THR:HB	1:D:721:LYS:HB2	1.93	0.50
1:D:474:GLY:HA2	1:D:476:GLY:O	2.11	0.50
1:A:313:LEU:O	1:A:325:MET:HA	2.10	0.50
1:B:547:TYR:HD1	1:B:549:GLY:H	1.54	0.50
1:C:597:ARG:NH1	1:C:682:HIS:HB2	2.25	0.50
1:D:272:ASN:ND2	1:D:274:ASP:N	2.59	0.50
1:A:383:HIS:CD2	1:A:399:LYS:HA	2.46	0.50
1:A:558:VAL:HG12	1:A:559:PHE:N	2.26	0.50
1:C:195:TYR:CD1	1:C:195:TYR:N	2.79	0.50
1:C:761:GLN:NE2	1:C:762:CYS:CA	2.74	0.50
1:A:692:ALA:O	1:A:695:PHE:HB2	2.11	0.50
1:B:135:TYR:C	1:B:135:TYR:CD2	2.85	0.50
1:C:258:LYS:HD2	1:D:248:TYR:CD2	2.46	0.50
1:D:649:CYS:HA	1:D:699:GLU:O	2.11	0.50
1:A:607:ILE:O	1:A:610:ALA:HB3	2.11	0.50
1:B:207:VAL:HG12	1:B:208:PHE:HD1	1.76	0.50
1:D:243:ASP:HB3	3:D:796:HOH:O	2.11	0.50
1:D:709:ASP:O	1:D:712:HIS:CE1	2.65	0.50
1:A:76:ILE:CD1	1:A:105:TYR:CZ	2.95	0.50
1:D:175:LYS:HD3	1:D:178:PRO:HA	1.93	0.50
1:A:542:LEU:C	1:A:542:LEU:HD23	2.32	0.50
1:A:93:SER:O	1:A:96:ASP:HB2	2.11	0.50
1:B:614:SER:HA	1:B:619:VAL:HB	1.92	0.50
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.94	0.50
1:C:518:ILE:O	1:C:519:LEU:HD23	2.11	0.50
1:D:388:GLN:HB2	1:D:391:LYS:HB2	1.92	0.50
1:D:414:TYR:CD2	1:D:433:LYS:HG2	2.47	0.50
1:A:676:PRO:HG2	1:A:677:GLU:H	1.77	0.50
1:A:71:LYS:HG3	1:A:76:ILE:CG1	2.42	0.50
1:B:341:VAL:O	1:B:344:GLN:HB2	2.11	0.50
1:A:664:SER:O	1:A:668:GLU:HG3	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:TYR:HE1	1:B:549:GLY:HA3	1.77	0.49
1:C:701:LEU:HD13	1:C:731:GLN:CB	2.37	0.49
1:B:377:ASN:OD1	1:B:379:GLU:N	2.44	0.49
1:D:236:ILE:CG2	1:D:254:VAL:HG13	2.42	0.49
1:D:681:ASP:HB3	3:D:852:HOH:O	2.12	0.49
1:A:429:ARG:NH1	1:A:429:ARG:CG	2.70	0.49
1:B:316:LEU:CD2	1:B:320:GLN:HG2	2.42	0.49
1:C:385:CYS:HA	1:C:396:PHE:HA	1.93	0.49
1:C:68:TYR:CE1	1:C:79:PHE:CD2	3.01	0.49
1:D:214:LEU:CD1	1:D:223:LEU:HD11	2.41	0.49
1:D:751:ILE:CG2	1:D:752:TYR:N	2.75	0.49
1:B:535:ASP:C	1:B:537:SER:H	2.16	0.49
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.33	0.49
1:C:316:LEU:CD1	1:C:323:SER:HB3	2.42	0.49
1:C:408:GLU:N	1:C:416:TYR:O	2.39	0.49
1:C:512:LYS:HD3	3:C:818:HOH:O	2.12	0.49
1:C:61:ARG:O	1:C:63:ILE:HG23	2.12	0.49
1:D:98:PHE:HE1	1:D:142:LEU:HD21	1.76	0.49
1:A:588:ASP:O	1:A:592:HIS:HB2	2.12	0.49
1:A:74:ASN:HB2	1:A:92:ASN:HB2	1.95	0.49
1:B:134:ILE:O	1:B:142:LEU:HD12	2.12	0.49
1:B:199:THR:HA	1:B:228:PHE:CD2	2.47	0.49
1:B:388:GLN:HG2	1:B:391:LYS:CE	2.42	0.49
1:B:534:PHE:HA	1:B:540:TYR:OH	2.12	0.49
1:B:60:LEU:O	1:B:60:LEU:HD12	2.12	0.49
1:B:73:GLU:O	1:B:75:ASN:ND2	2.46	0.49
1:C:175:LYS:NZ	1:C:180:LEU:O	2.46	0.49
1:A:613:PHE:O	1:A:615:LYS:N	2.46	0.49
1:B:486:VAL:CG1	1:B:487:ASN:N	2.75	0.49
1:B:542:LEU:HD23	1:B:543:LEU:N	2.28	0.49
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.94	0.49
1:C:597:ARG:HA	1:C:682:HIS:CD2	2.47	0.49
1:C:728:VAL:HG22	1:C:728:VAL:O	2.12	0.49
1:D:370:SER:OG	1:D:386:TYR:HE1	1.95	0.49
1:A:142:LEU:O	1:A:143:ILE:O	2.31	0.49
1:A:175:LYS:HD2	3:A:812:HOH:O	2.12	0.49
1:A:716:SER:O	1:A:719:ILE:N	2.45	0.49
1:B:636:THR:HG21	1:B:651:ILE:O	2.13	0.49
1:D:159:PRO:HD3	1:D:216:TRP:CG	2.47	0.49
1:D:51:ASN:O	1:D:54:ARG:HD3	2.13	0.49
1:D:631:TYR:HB2	2:D:767:13Z:F1	2.03	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ASP:HB3	1:B:441:LYS:HG3	1.95	0.49
1:C:345:HIS:HE1	1:C:389:ILE:O	1.95	0.49
1:C:471:ARG:HH11	1:C:471:ARG:HG3	1.77	0.49
1:D:125:ARG:HG2	1:D:126:HIS:NE2	2.27	0.49
1:D:146:GLU:HB3	1:D:180:LEU:O	2.13	0.49
1:A:626:ILE:O	1:A:626:ILE:HG23	2.12	0.49
1:C:755:MET:O	1:C:759:ILE:HG12	2.12	0.49
1:D:257:PRO:O	1:D:663:ASP:HA	2.12	0.49
1:A:225:TYR:CZ	1:A:269:PHE:HB2	2.48	0.49
1:B:184:ARG:HD3	1:B:186:THR:O	2.12	0.49
1:B:241:TYR:O	1:B:242:SER:HB3	2.13	0.49
1:B:289:ALA:HB2	1:B:315:TRP:CZ3	2.48	0.49
1:C:454:CYS:HA	1:C:474:GLY:O	2.13	0.49
1:D:562:ASN:HB2	3:D:845:HOH:O	2.13	0.49
1:D:704:HIS:NE2	1:D:711:VAL:O	2.45	0.49
1:A:242:SER:HB3	1:A:246:LEU:HD22	1.94	0.48
1:C:300:LEU:HD13	1:C:315:TRP:CZ3	2.48	0.48
1:C:654:ALA:HA	1:C:704:HIS:CE1	2.47	0.48
1:C:61:ARG:O	1:C:68:TYR:HA	2.12	0.48
1:A:145:GLU:O	1:A:146:GLU:HB2	2.13	0.48
1:A:199:THR:HG21	1:A:208:PHE:HD2	1.78	0.48
1:A:293:MET:HG2	1:A:315:TRP:HB3	1.95	0.48
1:B:169:ASN:N	1:B:169:ASN:HD22	2.10	0.48
1:B:208:PHE:N	1:B:208:PHE:HD1	2.11	0.48
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.42	0.48
1:B:80:ASN:OD1	1:B:82:GLU:N	2.46	0.48
1:C:249:PRO:HD3	1:D:714:GLN:NE2	2.27	0.48
1:A:138:ASN:O	1:A:140:ARG:HG2	2.12	0.48
1:A:478:PRO:HB2	1:A:497:ASN:HD21	1.77	0.48
1:C:374:ILE:HD11	1:C:404:VAL:HG12	1.95	0.48
1:D:108:SER:HB3	1:D:157:TRP:CZ2	2.48	0.48
1:D:169:ASN:O	1:D:170:ASN:HB2	2.12	0.48
1:A:347:GLU:OE1	1:A:373:LYS:HE3	2.13	0.48
1:A:60:LEU:O	1:A:60:LEU:HD12	2.13	0.48
1:A:73:GLU:C	1:A:75:ASN:H	2.15	0.48
1:B:156:THR:HG21	1:B:214:LEU:CD1	2.43	0.48
1:B:89:PHE:CD1	1:B:89:PHE:C	2.87	0.48
1:D:224:ALA:CB	1:D:270:VAL:HG22	2.44	0.48
1:D:501:ASP:O	1:D:505:GLN:HG2	2.14	0.48
1:D:620:ASP:OD2	1:D:623:ARG:HD3	2.12	0.48
1:A:498:SER:O	1:A:501:ASP:HB3	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:VAL:CG1	1:A:559:PHE:N	2.77	0.48
1:B:207:VAL:HG12	1:B:208:PHE:CD1	2.49	0.48
1:B:370:SER:HB2	1:B:387:PHE:O	2.13	0.48
1:B:386:TYR:O	1:B:394:CYS:HB2	2.12	0.48
1:B:513:LYS:HZ3	1:B:515:ASP:HB2	1.79	0.48
1:B:657:SER:O	1:B:688:VAL:HG23	2.13	0.48
1:B:84:GLY:HA3	1:B:492:ARG:HH12	1.71	0.48
1:C:301:CYS:SG	1:C:316:LEU:HB2	2.54	0.48
1:C:486:VAL:HG13	1:C:487:ASN:N	2.28	0.48
1:D:175:LYS:HE3	1:D:180:LEU:O	2.13	0.48
1:D:382:ARG:HD2	1:D:403:GLU:OE2	2.13	0.48
1:A:367:ASP:OD1	1:A:369:ASN:N	2.43	0.48
1:A:48:TYR:CD2	1:A:49:LEU:HD23	2.48	0.48
1:A:481:THR:HG22	1:A:493:VAL:HG22	1.96	0.48
1:B:666:TYR:C	1:B:666:TYR:CD1	2.86	0.48
1:C:472:CYS:O	1:C:478:PRO:HA	2.14	0.48
1:C:73:GLU:O	1:C:75:ASN:ND2	2.43	0.48
1:B:733:MET:HG3	1:B:735:TYR:CE2	2.49	0.48
1:D:259:ALA:HB3	1:D:660:GLU:HA	1.96	0.48
1:D:293:MET:HG3	1:D:315:TRP:HB2	1.95	0.48
1:A:658:ARG:HD3	1:A:660:GLU:HB2	1.94	0.48
1:B:562:ASN:HB2	3:B:830:HOH:O	2.14	0.48
1:C:553:GLN:HA	1:C:579:ASP:OD1	2.14	0.48
1:C:675:THR:HB	1:C:676:PRO:HD2	1.95	0.48
1:D:581:ARG:HB2	1:D:605:ASP:OD2	2.14	0.48
1:D:68:TYR:CD1	1:D:68:TYR:O	2.66	0.48
1:A:334:SER:C	1:A:336:ARG:H	2.16	0.48
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.48
1:B:422:TYR:CD1	1:B:447:CYS:SG	3.07	0.48
1:B:55:LEU:HD11	1:B:478:PRO:HD2	1.96	0.48
1:B:644:SER:O	1:B:646:VAL:N	2.47	0.48
1:C:135:TYR:HD1	1:C:142:LEU:HD13	1.78	0.48
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.95	0.48
1:C:45:LEU:HD13	1:C:566:TYR:CD2	2.48	0.48
1:B:170:ASN:O	1:B:196:ASN:HB2	2.14	0.48
1:C:107:ILE:CD1	1:C:114:ILE:HD12	2.44	0.48
1:D:219:ASN:OD1	1:D:219:ASN:C	2.53	0.48
1:D:341:VAL:HG13	1:D:342:ALA:N	2.28	0.48
1:D:755:MET:O	1:D:759:ILE:HG12	2.14	0.48
1:A:615:LYS:O	1:A:616:MET:C	2.52	0.47
1:C:233:VAL:HG12	1:C:234:PRO:O	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:GLN:HA	1:C:308:GLN:OE1	2.14	0.47
1:C:627:TRP:HB2	1:C:651:ILE:HB	1.96	0.47
1:D:99:GLY:O	1:D:100:HIS:CG	2.67	0.47
1:D:516:PHE:CD2	1:D:523:LYS:HD3	2.49	0.47
1:A:150:ASN:O	1:A:151:ASN:CB	2.59	0.47
1:A:154:TRP:CZ3	1:A:156:THR:CG2	2.98	0.47
1:A:546:VAL:HG12	1:A:627:TRP:O	2.13	0.47
1:A:67:GLU:HA	1:A:79:PHE:O	2.14	0.47
1:B:113:PHE:CD2	1:B:178:PRO:HG2	2.48	0.47
1:B:445:LEU:HD23	1:B:445:LEU:N	2.29	0.47
1:B:487:ASN:C	1:B:487:ASN:HD22	2.17	0.47
1:B:500:LEU:HG	1:B:504:LEU:HD12	1.96	0.47
1:B:763:PHE:HB2	1:B:765:LEU:CD2	2.44	0.47
1:C:107:ILE:HG22	1:C:108:SER:O	2.14	0.47
1:D:75:ASN:OD1	1:D:77:LEU:HD11	2.14	0.47
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.45	0.47
1:C:74:ASN:C	1:C:92:ASN:HB3	2.35	0.47
1:A:468:TYR:O	1:A:483:HIS:N	2.36	0.47
1:A:753:THR:O	1:A:757:HIS:CD2	2.67	0.47
1:B:319:ILE:O	1:B:321:ASN:N	2.43	0.47
1:C:309:GLU:HB3	1:C:330:TYR:HB3	1.96	0.47
1:C:75:ASN:HD21	1:C:92:ASN:CG	2.18	0.47
1:B:136:ASP:HB3	1:B:139:LYS:HG2	1.96	0.47
1:C:510:PRO:HB2	1:C:530:LEU:O	2.14	0.47
1:D:156:THR:HG23	1:D:165:ALA:O	2.15	0.47
1:A:115:LEU:HD21	1:A:155:VAL:HG11	1.97	0.47
1:A:124:TRP:HA	1:A:124:TRP:CE3	2.48	0.47
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.50	0.47
1:B:369:ASN:C	1:B:389:ILE:HG23	2.34	0.47
1:B:39:THR:HG22	1:B:39:THR:O	2.13	0.47
1:B:454:CYS:HA	1:B:474:GLY:O	2.15	0.47
1:B:477:LEU:HD12	1:B:501:ASP:HB2	1.97	0.47
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.49	0.47
1:D:487:ASN:N	1:D:487:ASN:HD22	2.09	0.47
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.79	0.47
1:A:465:ALA:O	1:A:485:SER:OG	2.21	0.47
1:A:51:ASN:O	1:A:52:THR:C	2.51	0.47
1:B:57:LEU:HB3	1:B:480:TYR:OH	2.15	0.47
1:C:124:TRP:HA	1:C:124:TRP:CE3	2.50	0.47
1:D:173:TYR:CD2	1:D:184:ARG:HA	2.50	0.47
1:D:484:SER:HB2	1:D:491:LEU:HD21	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:ASN:C	1:D:522:THR:H	2.16	0.47
1:A:509:MET:HE3	1:A:510:PRO:HD2	1.97	0.47
1:B:206:GLU:OE2	1:B:666:TYR:HB2	2.15	0.47
1:C:159:PRO:HD3	1:C:216:TRP:HB2	1.95	0.47
1:C:319:ILE:HG13	1:C:319:ILE:O	2.15	0.47
1:C:320:GLN:OE1	1:C:669:ARG:HD3	2.14	0.47
1:C:369:ASN:HA	1:C:389:ILE:CG2	2.44	0.47
1:C:50:LYS:HE3	1:C:749:GLN:OE1	2.15	0.47
1:D:293:MET:HE3	1:D:324:VAL:HG23	1.97	0.47
1:D:356:ARG:HD3	1:D:551:CYS:SG	2.54	0.47
1:A:113:PHE:CE2	1:A:178:PRO:HG2	2.50	0.47
1:A:499:ALA:O	1:A:500:LEU:C	2.53	0.47
1:B:43:TYR:CD2	1:B:565:THR:HG22	2.49	0.47
1:C:482:LEU:C	1:C:483:HIS:CD2	2.87	0.47
1:D:154:TRP:NE1	1:D:212:SER:HB2	2.30	0.47
1:A:122:LYS:NZ	1:A:124:TRP:O	2.31	0.47
1:A:135:TYR:OH	1:A:140:ARG:NE	2.48	0.47
1:A:634:TYR:CD1	1:A:656:VAL:O	2.68	0.47
1:B:453:ARG:HG2	1:B:454:CYS:SG	2.55	0.47
1:D:208:PHE:O	1:D:209:SER:HB3	2.14	0.47
1:D:571:GLU:O	1:D:572:ASN:C	2.53	0.47
1:A:154:TRP:CZ3	1:A:156:THR:HB	2.50	0.47
1:A:404:VAL:HG13	1:A:417:TYR:HD1	1.80	0.47
1:A:751:ILE:O	1:A:751:ILE:HG12	2.15	0.47
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.30	0.47
1:B:620:ASP:O	1:B:621:ASN:C	2.53	0.47
1:D:306:ALA:HB3	1:D:310:ARG:O	2.15	0.47
1:B:285:ILE:HG21	1:B:336:ARG:HA	1.95	0.46
1:A:279:VAL:HG12	1:A:280:THR:OG1	2.15	0.46
1:A:543:LEU:HD11	1:A:627:TRP:HD1	1.80	0.46
1:A:651:ILE:CD1	1:A:755:MET:HE2	2.45	0.46
1:B:519:LEU:O	1:B:522:THR:HG23	2.15	0.46
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.62	0.46
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.50	0.46
1:C:411:THR:OG1	1:C:414:TYR:N	2.47	0.46
1:D:320:GLN:OE1	1:D:669:ARG:HD3	2.15	0.46
1:D:463:LYS:HB3	1:D:464:GLU:OE2	2.14	0.46
1:D:764:SER:OG	1:D:764:SER:O	2.32	0.46
1:A:196:ASN:OD1	1:A:227:GLN:NE2	2.46	0.46
1:A:314:GLN:HG2	1:A:325:MET:HB2	1.97	0.46
1:B:105:TYR:HD2	1:B:107:ILE:CD1	2.29	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASN:ND2	1:B:318:ARG:CZ	2.78	0.46
1:C:310:ARG:NH1	1:C:368:GLY:O	2.48	0.46
1:C:374:ILE:HD11	1:C:404:VAL:CG1	2.45	0.46
1:C:375:ILE:O	1:C:382:ARG:HA	2.16	0.46
1:C:81:ALA:O	1:C:492:ARG:NH2	2.47	0.46
1:D:530:LEU:HA	1:D:531:PRO:HD3	1.81	0.46
1:A:664:SER:OG	1:A:665:VAL:N	2.48	0.46
1:A:631:TYR:HB2	2:A:767:13Z:F1	2.05	0.46
1:B:105:TYR:CD2	1:B:107:ILE:CD1	2.99	0.46
1:B:187:TRP:CH2	1:B:281:ASN:OD1	2.69	0.46
1:C:105:TYR:HA	1:C:115:LEU:O	2.16	0.46
1:C:118:TYR:N	1:C:118:TYR:CD1	2.83	0.46
1:C:69:LEU:HD23	1:C:78:VAL:HA	1.96	0.46
1:C:701:LEU:CD1	1:C:731:GLN:HB2	2.37	0.46
1:D:374:ILE:HD11	1:D:404:VAL:HG12	1.97	0.46
1:D:586:GLN:HB2	3:D:843:HOH:O	2.15	0.46
1:A:542:LEU:O	1:A:624:ILE:HA	2.15	0.46
1:B:170:ASN:OD1	1:B:170:ASN:N	2.48	0.46
1:B:508:GLN:HB3	1:B:532:PRO:HG2	1.97	0.46
1:B:519:LEU:O	1:B:521:GLU:N	2.49	0.46
1:D:72:GLN:NE2	1:D:77:LEU:HD22	2.30	0.46
1:A:712:HIS:C	1:A:714:GLN:N	2.67	0.46
1:B:107:ILE:HA	1:B:114:ILE:HA	1.98	0.46
1:B:527:GLN:HG3	1:B:527:GLN:O	2.16	0.46
1:B:550:PRO:O	1:B:551:CYS:HB3	2.16	0.46
1:D:55:LEU:CD2	1:D:561:LEU:HD12	2.46	0.46
1:A:157:TRP:O	1:A:216:TRP:NE1	2.49	0.46
1:A:383:HIS:HB3	1:A:398:THR:OG1	2.15	0.46
1:B:500:LEU:HG	1:B:504:LEU:CD1	2.46	0.46
1:C:201:TRP:CH2	1:C:205:GLU:HG2	2.51	0.46
1:C:216:TRP:HZ3	1:C:273:THR:HG21	1.80	0.46
1:C:621:ASN:H	1:C:621:ASN:ND2	2.14	0.46
1:A:230:ASP:O	1:A:233:VAL:HB	2.16	0.46
1:A:312:SER:HA	1:A:326:ASP:O	2.15	0.46
1:A:68:TYR:CE1	1:A:79:PHE:CB	2.98	0.46
1:B:115:LEU:HB2	1:B:157:TRP:HZ2	1.81	0.46
1:B:317:ARG:O	1:B:319:ILE:N	2.48	0.46
1:C:215:TRP:N	1:C:215:TRP:CE3	2.84	0.46
1:C:530:LEU:HD13	1:C:534:PHE:CD2	2.51	0.46
1:D:307:THR:OG1	1:D:310:ARG:N	2.49	0.46
1:D:532:PRO:O	1:D:533:HIS:C	2.55	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ASN:OD1	1:D:83:TYR:N	2.49	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.50	0.46
1:A:325:MET:HE1	1:A:362:PRO:HG3	1.97	0.46
1:A:728:VAL:HG23	1:A:729:ASP:O	2.15	0.46
1:A:77:LEU:HD23	1:A:77:LEU:N	2.31	0.46
1:B:317:ARG:O	1:B:318:ARG:C	2.54	0.46
1:B:532:PRO:O	1:B:533:HIS:HB2	2.15	0.46
1:D:224:ALA:HB2	1:D:270:VAL:HG22	1.98	0.46
1:D:709:ASP:OD1	1:D:709:ASP:N	2.48	0.46
1:A:228:PHE:HA	1:A:265:THR:O	2.16	0.46
1:B:246:LEU:HD11	1:B:248:TYR:O	2.15	0.46
1:C:109:PRO:HG2	1:C:158:SER:O	2.16	0.46
1:D:253:ARG:NH1	1:D:253:ARG:CB	2.79	0.46
1:A:610:ALA:O	1:A:611:ARG:C	2.53	0.45
1:A:742:ILE:HD13	1:A:751:ILE:HD12	1.97	0.45
1:B:43:TYR:CD2	1:B:565:THR:CG2	2.99	0.45
1:B:598:LEU:O	1:B:682:HIS:NE2	2.44	0.45
1:B:633:GLY:C	1:B:655:PRO:HB3	2.36	0.45
1:B:81:ALA:HB3	1:B:467:TYR:CE2	2.50	0.45
1:D:139:LYS:HG2	1:D:141:GLN:CB	2.46	0.45
1:D:173:TYR:CE2	1:D:184:ARG:CG	2.80	0.45
1:D:47:ASP:HA	1:D:52:THR:HG23	1.99	0.45
1:A:208:PHE:O	1:A:210:ALA:N	2.49	0.45
1:A:381:TYR:CE2	1:A:401:THR:CA	2.98	0.45
1:A:533:HIS:O	1:A:534:PHE:C	2.55	0.45
1:B:206:GLU:OE1	1:B:206:GLU:HA	2.16	0.45
1:B:237:GLU:CG	1:B:253:ARG:HG2	2.46	0.45
1:C:244:GLU:OE2	1:D:658:ARG:NH2	2.48	0.45
1:D:414:TYR:CD2	1:D:433:LYS:CG	3.00	0.45
1:D:597:ARG:HA	1:D:682:HIS:CD2	2.51	0.45
1:A:256:TYR:O	1:B:248:TYR:OH	2.28	0.45
1:A:314:GLN:HE22	1:A:361:GLU:HA	1.80	0.45
1:B:422:TYR:CE1	1:B:447:CYS:HB3	2.51	0.45
1:D:57:LEU:N	1:D:57:LEU:HD12	2.28	0.45
1:D:76:ILE:O	1:D:89:PHE:N	2.49	0.45
1:A:676:PRO:HG2	1:A:677:GLU:N	2.31	0.45
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.99	0.45
1:B:52:THR:HG22	3:B:816:HOH:O	2.16	0.45
1:C:507:VAL:CG2	1:C:508:GLN:N	2.79	0.45
1:A:114:ILE:HG22	1:A:137:LEU:HG	1.99	0.45
1:A:513:LYS:O	1:A:527:GLN:HA	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:C	1:A:60:LEU:HD12	2.37	0.45
1:B:250:LYS:HG2	1:B:251:THR:N	2.31	0.45
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.51	0.45
1:C:364:PHE:HA	1:C:371:PHE:CB	2.47	0.45
1:D:331:ASP:O	1:D:335:GLY:N	2.37	0.45
1:A:290:PRO:HD3	1:A:326:ASP:OD2	2.17	0.45
1:D:95:PHE:CD1	1:D:116:LEU:HD11	2.52	0.45
1:A:138:ASN:C	1:A:140:ARG:N	2.70	0.45
1:A:113:PHE:CE1	1:A:143:ILE:HD11	2.52	0.45
1:A:49:LEU:HB3	1:A:749:GLN:HG2	1.98	0.45
1:A:738:GLU:OE2	1:A:744:SER:OG	2.34	0.45
1:B:516:PHE:HA	1:B:526:TYR:HD2	1.82	0.45
1:D:343:ARG:NE	1:D:389:ILE:HD12	2.32	0.45
1:D:459:VAL:CG1	1:D:461:PHE:HE1	2.30	0.45
1:D:763:PHE:O	1:D:764:SER:C	2.55	0.45
1:A:76:ILE:HD11	1:A:105:TYR:CZ	2.51	0.45
1:A:233:VAL:HG22	1:A:262:VAL:O	2.17	0.45
1:A:426:PRO:HD2	1:A:525:TRP:CE2	2.52	0.45
1:B:58:TYR:CE2	1:B:494:LEU:HB3	2.52	0.45
1:B:547:TYR:CE1	1:B:549:GLY:HA3	2.50	0.45
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.97	0.45
1:C:367:ASP:OD1	1:C:369:ASN:N	2.50	0.45
1:C:558:VAL:HG12	1:C:559:PHE:N	2.32	0.45
1:D:164:LEU:HA	1:D:164:LEU:HD23	1.80	0.45
1:A:285:ILE:HG23	1:A:336:ARG:HE	1.82	0.45
1:A:490:GLY:O	1:A:491:LEU:C	2.55	0.45
1:B:215:TRP:CH2	1:B:303:VAL:HG21	2.52	0.45
1:B:627:TRP:O	1:B:627:TRP:CG	2.69	0.45
1:B:742:ILE:HD12	1:B:751:ILE:HD12	1.99	0.45
1:C:611:ARG:HG2	1:C:615:LYS:HZ2	1.80	0.45
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.51	0.45
1:D:422:TYR:CD2	1:D:423:LYS:HG3	2.52	0.45
1:A:202:VAL:CG1	1:A:203:TYR:N	2.80	0.44
1:A:562:ASN:OD1	1:A:564:ALA:N	2.50	0.44
1:A:620:ASP:OD2	1:A:623:ARG:CD	2.64	0.44
1:B:316:LEU:HD21	1:B:320:GLN:HB3	1.99	0.44
1:B:535:ASP:OD2	1:B:535:ASP:C	2.54	0.44
1:B:662:TYR:CE2	2:B:767:13Z:H4	2.52	0.44
1:B:83:TYR:HB2	1:B:85:ASN:OD1	2.17	0.44
1:C:148:ILE:HD12	1:C:148:ILE:N	2.31	0.44
1:C:581:ARG:CZ	1:C:601:PHE:CD1	3.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:GLU:N	1:C:602:GLU:OE2	2.48	0.44
1:D:160:VAL:HG12	1:D:161:GLY:N	2.32	0.44
1:D:39:THR:HB	3:D:768:HOH:O	2.16	0.44
1:D:60:LEU:O	1:D:60:LEU:HD12	2.16	0.44
1:A:288:THR:HG22	3:A:815:HOH:O	2.16	0.44
1:C:175:LYS:HG3	1:C:182:SER:HA	2.00	0.44
1:C:272:ASN:OD1	1:C:274:ASP:N	2.50	0.44
1:C:300:LEU:HA	1:C:300:LEU:HD12	1.86	0.44
1:C:544:LEU:HD12	1:C:576:ALA:O	2.17	0.44
1:D:451:PRO:HA	3:D:859:HOH:O	2.16	0.44
1:A:417:TYR:CE2	1:A:432:TYR:HB2	2.51	0.44
1:B:113:PHE:CE1	1:B:136:ASP:HA	2.52	0.44
1:C:257:PRO:HG2	1:C:664:SER:OG	2.17	0.44
1:C:364:PHE:HA	1:C:371:PHE:HB3	2.00	0.44
1:C:747:ALA:O	1:C:751:ILE:HG22	2.17	0.44
1:D:662:TYR:CE2	2:D:767:13Z:H4	2.52	0.44
1:B:513:LYS:HZ2	1:B:515:ASP:HB2	1.81	0.44
1:B:662:TYR:HB3	1:B:667:THR:OG1	2.18	0.44
1:C:137:LEU:O	1:C:140:ARG:CD	2.62	0.44
1:D:137:LEU:N	1:D:137:LEU:CD2	2.79	0.44
1:D:258:LYS:NZ	1:D:712:HIS:HD2	2.16	0.44
1:D:636:THR:HG22	1:D:640:LEU:HD12	2.00	0.44
1:D:63:ILE:HG22	1:D:67:GLU:O	2.16	0.44
1:D:72:GLN:O	1:D:74:ASN:N	2.50	0.44
1:D:740:HIS:NE2	2:D:767:13Z:N2	2.66	0.44
1:A:372:TYR:CD2	1:A:415:LEU:HD12	2.52	0.44
1:A:64:SER:C	1:A:463:LYS:HG2	2.38	0.44
1:A:477:LEU:HD22	1:A:500:LEU:HD23	1.98	0.44
1:A:723:LEU:HD22	1:A:728:VAL:HG11	1.99	0.44
1:B:73:GLU:O	1:B:74:ASN:HB2	2.17	0.44
1:C:153:GLN:HE22	1:C:170:ASN:ND2	2.16	0.44
1:C:302:ASP:OD1	1:C:303:VAL:N	2.51	0.44
1:C:317:ARG:O	1:C:318:ARG:C	2.55	0.44
1:D:594:ILE:CG2	1:D:601:PHE:HB2	2.47	0.44
1:A:477:LEU:CD1	1:A:500:LEU:HD23	2.44	0.44
1:A:82:GLU:OE1	1:A:467:TYR:CE1	2.70	0.44
1:B:115:LEU:CG	1:B:132:TYR:HD2	2.31	0.44
1:B:136:ASP:O	1:B:137:LEU:C	2.56	0.44
1:B:268:PHE:CD2	1:B:313:LEU:HD11	2.52	0.44
1:B:85:ASN:N	1:B:85:ASN:OD1	2.50	0.44
1:C:272:ASN:OD1	1:C:272:ASN:C	2.56	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:HH21	1:C:343:ARG:HH12	1.66	0.44
1:C:630:SER:O	1:C:655:PRO:HA	2.18	0.44
1:D:102:ILE:HD13	1:D:116:LEU:HD22	2.00	0.44
1:D:208:PHE:O	1:D:209:SER:CB	2.66	0.44
1:A:235:LEU:HD21	1:A:255:PRO:HG3	2.00	0.44
1:B:115:LEU:HB2	1:B:157:TRP:CZ2	2.51	0.44
1:C:124:TRP:HA	1:C:124:TRP:HE3	1.82	0.44
1:C:312:SER:C	1:C:313:LEU:HD12	2.37	0.44
1:C:487:ASN:O	1:C:488:ASP:C	2.55	0.44
1:D:112:GLN:HB3	1:D:113:PHE:CE2	2.52	0.44
1:D:456:TYR:HB2	1:D:557:THR:OG1	2.17	0.44
1:A:125:ARG:NH2	1:A:205:GLU:OE2	2.51	0.44
1:B:428:GLY:C	1:B:429:ARG:HG2	2.38	0.44
1:C:418:ILE:HA	1:C:430:ASN:O	2.18	0.44
1:D:266:VAL:HG22	1:D:267:LYS:N	2.33	0.44
1:D:761:GLN:HB3	1:D:761:GLN:HE21	1.57	0.44
1:A:280:THR:HG22	1:A:281:ASN:N	2.33	0.44
1:A:730:PHE:CD1	1:A:731:GLN:O	2.68	0.44
1:B:200:ASP:OD2	1:B:230:ASP:OD2	2.36	0.44
1:B:546:VAL:HB	1:B:606:GLN:OE1	2.18	0.44
1:C:107:ILE:HD11	1:C:114:ILE:HD12	1.99	0.44
1:C:658:ARG:HH22	1:C:684:ARG:CD	2.30	0.44
1:C:75:ASN:OD1	1:C:92:ASN:OD1	2.36	0.44
1:D:76:ILE:O	1:D:89:PHE:HB3	2.18	0.44
1:A:267:LYS:HB3	1:A:269:PHE:CE1	2.53	0.43
1:A:658:ARG:CB	1:A:687:THR:HG22	2.48	0.43
1:A:738:GLU:CD	1:A:744:SER:OG	2.56	0.43
1:A:79:PHE:CE1	1:A:86:SER:HB3	2.52	0.43
1:C:608:GLU:O	1:C:612:GLN:HG3	2.17	0.43
1:C:751:ILE:HG23	1:C:752:TYR:N	2.33	0.43
1:D:68:TYR:C	1:D:68:TYR:CD1	2.91	0.43
1:D:715:GLN:O	1:D:719:ILE:HG13	2.18	0.43
1:D:73:GLU:CD	1:D:73:GLU:H	2.20	0.43
1:B:382:ARG:HG2	1:B:382:ARG:HH11	1.83	0.43
1:B:487:ASN:HD22	1:B:488:ASP:N	2.17	0.43
1:B:543:LEU:HD12	1:B:625:ALA:O	2.18	0.43
1:C:175:LYS:HG3	1:C:182:SER:CA	2.48	0.43
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.17	0.43
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.53	0.43
1:D:546:VAL:HG21	1:D:606:GLN:HG2	2.00	0.43
1:D:631:TYR:O	1:D:634:TYR:HB3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:SER:C	1:B:132:TYR:CD1	2.92	0.43
1:B:658:ARG:CB	1:B:687:THR:HG22	2.42	0.43
1:C:331:ASP:HB3	1:C:334:SER:HB3	2.00	0.43
1:C:40:ARG:NH1	1:C:505:GLN:O	2.48	0.43
1:C:662:TYR:CE2	2:C:767:13Z:H4	2.53	0.43
1:D:143:ILE:CG2	1:D:179:ASN:OD1	2.53	0.43
1:D:640:LEU:CD2	1:D:698:VAL:HG21	2.48	0.43
1:A:98:PHE:HE1	1:A:142:LEU:HD11	1.83	0.43
1:A:170:ASN:N	1:A:170:ASN:HD22	2.15	0.43
1:A:244:GLU:HA	1:B:718:GLN:HE22	1.82	0.43
1:A:554:LYS:H	1:A:579:ASP:CG	2.21	0.43
1:A:623:ARG:NH2	1:A:763:PHE:O	2.45	0.43
1:B:520:ASN:O	1:B:521:GLU:HB2	2.18	0.43
1:C:224:ALA:HB2	1:C:270:VAL:HG13	1.99	0.43
1:C:305:TRP:CE2	1:C:311:ILE:HD12	2.53	0.43
1:C:413:ASP:C	1:C:414:TYR:CD1	2.92	0.43
1:D:174:VAL:CG2	1:D:185:ILE:HD11	2.47	0.43
1:D:199:THR:CG2	1:D:208:PHE:CD2	3.02	0.43
1:D:520:ASN:O	1:D:522:THR:N	2.52	0.43
1:A:113:PHE:CD1	1:A:136:ASP:HA	2.53	0.43
1:A:486:VAL:CG1	1:A:487:ASN:N	2.82	0.43
1:B:516:PHE:HA	1:B:526:TYR:CD2	2.54	0.43
1:C:114:ILE:HG22	1:C:137:LEU:CD2	2.46	0.43
1:C:471:ARG:NH1	1:C:471:ARG:HG3	2.34	0.43
1:C:76:ILE:O	1:C:89:PHE:N	2.45	0.43
1:D:120:TYR:HA	1:D:130:ALA:HB2	1.99	0.43
1:D:310:ARG:NH1	1:D:310:ARG:HG3	2.33	0.43
1:D:662:TYR:HE1	1:D:710:ASN:OD1	2.02	0.43
1:A:547:TYR:CE1	2:A:767:13Z:H14A	2.53	0.43
1:C:457:TYR:CE1	1:C:472:CYS:HB2	2.52	0.43
1:C:600:THR:OG1	1:C:601:PHE:N	2.51	0.43
1:D:149:PRO:HB2	1:D:168:TRP:NE1	2.33	0.43
1:D:195:TYR:HB3	1:D:198:ILE:O	2.18	0.43
1:D:170:ASN:O	1:D:196:ASN:HB2	2.18	0.43
1:A:55:LEU:CD1	1:A:500:LEU:HD22	2.46	0.43
1:A:666:TYR:O	1:A:669:ARG:HB3	2.19	0.43
1:B:680:LEU:O	1:B:683:TYR:HB2	2.18	0.43
1:C:611:ARG:O	1:C:614:SER:HB3	2.19	0.43
1:C:661:TYR:CB	1:C:715:GLN:NE2	2.81	0.43
1:D:162:HIS:HD2	1:D:176:ILE:O	2.01	0.43
1:A:138:ASN:O	1:A:140:ARG:N	2.51	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HG22	1:A:152:THR:OG1	2.18	0.43
1:A:184:ARG:HD2	1:A:187:TRP:CD2	2.53	0.43
1:A:446:SER:HB2	1:A:457:TYR:CD2	2.54	0.43
1:B:272:ASN:HD22	1:B:274:ASP:H	1.64	0.43
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.53	0.43
1:C:756:SER:O	1:C:760:LYS:HG3	2.19	0.43
1:C:88:VAL:HG11	1:C:91:GLU:OE2	2.19	0.43
1:D:58:TYR:CE2	1:D:494:LEU:HB3	2.53	0.43
1:A:177:GLU:HB2	1:A:180:LEU:HD12	2.00	0.43
1:A:80:ASN:OD1	1:A:80:ASN:C	2.57	0.43
1:B:104:ASP:OD1	1:B:105:TYR:N	2.50	0.43
1:B:125:ARG:HG2	1:B:126:HIS:NE2	2.34	0.43
1:B:624:ILE:HG22	1:B:647:PHE:CD1	2.54	0.43
1:C:75:ASN:ND2	1:C:92:ASN:ND2	2.63	0.43
1:D:253:ARG:CB	1:D:253:ARG:HH11	2.31	0.43
1:A:76:ILE:HD13	1:A:105:TYR:CZ	2.54	0.43
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.88	0.43
1:B:190:LYS:HA	3:B:811:HOH:O	2.18	0.43
1:B:644:SER:C	1:B:646:VAL:H	2.21	0.43
1:B:73:GLU:OE2	1:B:73:GLU:N	2.52	0.43
1:C:171:ASP:OD2	1:C:186:THR:OG1	2.35	0.43
1:A:139:LYS:HB2	1:D:334:SER:HB3	2.00	0.42
1:A:174:VAL:HG23	1:A:185:ILE:CG1	2.48	0.42
1:A:310:ARG:NH1	1:A:368:GLY:O	2.52	0.42
1:A:384:ILE:HG13	1:A:404:VAL:HG21	2.01	0.42
1:A:516:PHE:CE2	1:A:523:LYS:HE3	2.53	0.42
1:A:380:GLY:O	1:A:587:GLY:HA2	2.19	0.42
1:B:154:TRP:CG	1:B:155:VAL:N	2.87	0.42
1:B:199:THR:HG22	1:B:228:PHE:CE2	2.54	0.42
1:B:546:VAL:CG2	1:B:547:TYR:N	2.82	0.42
1:B:608:GLU:O	1:B:612:GLN:HG2	2.19	0.42
1:B:651:ILE:HG21	1:B:755:MET:CE	2.48	0.42
1:B:676:PRO:HD2	1:B:677:GLU:OE2	2.18	0.42
1:B:637:SER:HB3	1:B:688:VAL:HG11	2.01	0.42
1:C:127:SER:CB	1:C:211:TYR:CG	3.02	0.42
1:C:369:ASN:HA	1:C:389:ILE:HG21	2.01	0.42
1:C:573:ILE:HD11	1:C:765:LEU:CD1	2.49	0.42
1:C:598:LEU:HD21	1:C:670:TYR:HB3	2.00	0.42
1:C:742:ILE:HG21	1:C:751:ILE:HD12	2.00	0.42
1:C:627:TRP:CE3	1:C:755:MET:HE3	2.54	0.42
1:A:397:ILE:CD1	1:A:434:ILE:HD13	2.44	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ARG:NH1	1:A:601:PHE:CD1	2.88	0.42
1:A:712:HIS:O	1:A:713:PHE:C	2.57	0.42
1:B:150:ASN:O	1:B:151:ASN:CB	2.64	0.42
1:C:123:GLN:HB3	1:C:124:TRP:H	1.69	0.42
1:C:235:LEU:HD21	1:C:255:PRO:HG3	2.00	0.42
1:D:135:TYR:HA	3:D:822:HOH:O	2.18	0.42
1:D:201:TRP:CH2	1:D:205:GLU:HG2	2.53	0.42
1:A:310:ARG:HD3	1:A:327:ILE:CG2	2.49	0.42
1:A:613:PHE:C	1:A:615:LYS:N	2.72	0.42
1:B:358:ARG:O	1:B:359:PRO:C	2.58	0.42
1:B:44:THR:O	1:B:47:ASP:HB2	2.19	0.42
1:B:765:LEU:H	1:B:765:LEU:CD2	2.29	0.42
1:C:376:SER:OG	1:C:380:GLY:HA2	2.19	0.42
1:C:482:LEU:HD12	1:C:482:LEU:HA	1.66	0.42
1:C:692:ALA:HB1	1:C:726:VAL:HG21	2.00	0.42
1:A:158:SER:HA	1:A:216:TRP:CD2	2.54	0.42
1:A:459:VAL:CG2	1:A:460:SER:N	2.80	0.42
1:B:115:LEU:HG	1:B:132:TYR:HD2	1.84	0.42
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.01	0.42
1:B:204:GLU:HG2	1:B:204:GLU:O	2.20	0.42
1:B:310:ARG:NH1	1:B:329:ASP:OD2	2.52	0.42
1:C:360:SER:OG	1:C:374:ILE:O	2.32	0.42
1:C:55:LEU:HD11	1:C:561:LEU:CD1	2.50	0.42
1:C:649:CYS:CB	1:C:699:GLU:HB2	2.48	0.42
1:D:142:LEU:HD12	1:D:142:LEU:HA	1.73	0.42
1:D:514:LEU:HD12	1:D:526:TYR:O	2.19	0.42
1:A:459:VAL:CG2	1:A:460:SER:H	2.29	0.42
1:A:526:TYR:CD1	1:A:526:TYR:C	2.92	0.42
1:B:194:ILE:HD13	1:B:229:ASN:HA	2.01	0.42
1:B:464:GLU:O	1:B:465:ALA:CB	2.67	0.42
1:B:514:LEU:CD2	1:B:557:THR:HG22	2.48	0.42
1:C:242:SER:HB3	1:C:246:LEU:HD23	2.02	0.42
1:C:249:PRO:HG3	1:D:714:GLN:NE2	2.34	0.42
1:C:519:LEU:HD21	1:C:612:GLN:HE22	1.82	0.42
1:C:621:ASN:HA	1:C:624:ILE:HD11	2.01	0.42
1:D:157:TRP:CE3	1:D:164:LEU:HD23	2.54	0.42
1:D:383:HIS:CE1	1:D:399:LYS:HA	2.55	0.42
1:D:384:ILE:CG1	1:D:404:VAL:HG11	2.50	0.42
1:D:594:ILE:HD12	1:D:598:LEU:HD23	2.00	0.42
1:D:75:ASN:HB3	1:D:92:ASN:H	1.83	0.42
1:A:293:MET:HE2	1:A:315:TRP:HB2	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:CA	1:A:92:ASN:HB3	2.48	0.42
1:B:517:ILE:HD12	1:B:612:GLN:HG3	2.01	0.42
1:B:651:ILE:HG21	1:B:755:MET:HE3	2.02	0.42
1:C:234:PRO:HB2	1:D:248:TYR:CE1	2.54	0.42
1:C:738:GLU:OE1	1:C:742:ILE:HA	2.20	0.42
1:D:229:ASN:HB3	1:D:265:THR:OG1	2.20	0.42
1:D:301:CYS:O	1:D:358:ARG:NH1	2.53	0.42
1:D:374:ILE:HD13	1:D:404:VAL:HG12	2.02	0.42
1:D:739:ASP:HB2	1:D:740:HIS:H	1.58	0.42
1:A:125:ARG:HH21	1:A:710:ASN:HD21	1.66	0.42
1:A:240:PHE:CE2	1:A:242:SER:HA	2.54	0.42
1:A:266:VAL:HG22	1:A:267:LYS:N	2.34	0.42
1:A:422:TYR:OH	1:A:423:LYS:HE3	2.20	0.42
1:B:317:ARG:C	1:B:319:ILE:N	2.72	0.42
1:B:519:LEU:O	1:B:520:ASN:C	2.58	0.42
1:D:526:TYR:HB2	1:D:577:SER:O	2.19	0.42
1:A:110:ASP:OD2	1:A:111:GLY:N	2.53	0.42
1:A:60:LEU:HD22	1:A:68:TYR:CD2	2.55	0.42
1:B:110:ASP:OD2	1:B:112:GLN:HB2	2.20	0.42
1:B:299:TYR:CE1	1:B:665:VAL:HG22	2.55	0.42
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.40	0.42
1:C:705:GLY:O	1:C:708:ASP:HB2	2.20	0.42
1:D:146:GLU:HG3	1:D:180:LEU:C	2.40	0.42
1:D:449:LEU:HA	1:D:449:LEU:HD23	1.73	0.42
1:A:136:ASP:OD1	1:A:138:ASN:HB2	2.20	0.42
1:B:168:TRP:CZ2	1:B:169:ASN:OD1	2.73	0.42
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.85	0.42
1:B:474:GLY:HA2	1:B:476:GLY:O	2.20	0.42
1:B:50:LYS:HA	1:B:50:LYS:HD3	1.82	0.42
1:C:562:ASN:O	1:C:565:THR:N	2.52	0.42
1:D:323:SER:OG	1:D:347:GLU:HB3	2.20	0.42
1:D:361:GLU:OE2	1:D:363:HIS:NE2	2.50	0.42
1:D:486:VAL:CG1	1:D:487:ASN:N	2.82	0.42
1:A:192:ASP:HA	1:A:195:TYR:OH	2.19	0.42
1:A:599:GLY:N	1:A:602:GLU:OE1	2.45	0.42
1:A:620:ASP:C	1:A:620:ASP:OD1	2.58	0.42
1:B:236:ILE:HG23	1:B:254:VAL:HG13	2.02	0.42
1:B:385:CYS:HA	1:B:396:PHE:HA	2.02	0.42
1:B:535:ASP:C	1:B:537:SER:N	2.72	0.42
1:B:546:VAL:HA	3:B:826:HOH:O	2.20	0.42
1:C:188:THR:HB	1:C:194:ILE:HG21	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:TYR:CD1	1:C:256:TYR:C	2.93	0.42
1:C:229:ASN:HB3	1:C:265:THR:OG1	2.20	0.42
1:C:433:LYS:O	1:C:433:LYS:HG3	2.19	0.42
1:D:634:TYR:HD1	1:D:656:VAL:O	2.02	0.42
1:A:115:LEU:HD21	1:A:155:VAL:CG1	2.50	0.41
1:A:159:PRO:HD3	1:A:216:TRP:HB3	2.02	0.41
1:B:614:SER:HB2	1:B:621:ASN:OD1	2.20	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.41
1:B:742:ILE:CD1	1:B:751:ILE:HD12	2.50	0.41
1:C:446:SER:HA	1:C:449:LEU:HG	2.02	0.41
1:C:468:TYR:O	1:C:482:LEU:HD12	2.20	0.41
1:C:547:TYR:O	1:C:549:GLY:N	2.53	0.41
1:C:551:CYS:HB2	1:C:591:MET:SD	2.59	0.41
1:C:263:ASN:HD21	1:C:664:SER:HB2	1.84	0.41
1:C:714:GLN:NE2	1:D:249:PRO:HD3	2.35	0.41
1:A:535:ASP:OD1	1:A:538:LYS:HE2	2.20	0.41
1:A:620:ASP:OD2	1:A:623:ARG:HD2	2.20	0.41
1:B:425:MET:HA	1:B:426:PRO:HD2	1.90	0.41
1:B:433:LYS:HB2	1:B:445:LEU:HD21	2.02	0.41
1:B:629:TRP:HA	1:B:653:VAL:O	2.20	0.41
1:B:707:ALA:HB2	1:B:737:ASP:HA	2.02	0.41
1:C:477:LEU:CD1	1:C:501:ASP:HB2	2.50	0.41
1:C:510:PRO:CB	1:C:530:LEU:O	2.68	0.41
1:D:167:VAL:HG13	1:D:171:ASP:O	2.20	0.41
1:D:51:ASN:OD1	1:D:54:ARG:HD2	2.20	0.41
1:A:148:ILE:HA	1:A:149:PRO:HD2	1.79	0.41
1:A:248:TYR:CD2	1:B:258:LYS:HD2	2.54	0.41
1:B:136:ASP:CB	1:B:139:LYS:HG2	2.51	0.41
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.56	0.41
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.90	0.41
1:C:177:GLU:HB2	1:C:180:LEU:HD12	2.01	0.41
1:C:336:ARG:NH1	1:C:336:ARG:CG	2.82	0.41
1:D:596:ARG:NH2	1:D:679:ASN:HB2	2.35	0.41
1:A:446:SER:HA	1:A:449:LEU:HD12	2.02	0.41
1:A:500:LEU:O	1:A:501:ASP:C	2.59	0.41
1:A:543:LEU:HD23	1:A:567:LEU:HD13	2.03	0.41
1:B:146:GLU:OE1	1:B:181:PRO:HA	2.20	0.41
1:B:596:ARG:HA	1:B:670:TYR:O	2.20	0.41
1:D:105:TYR:HD2	1:D:107:ILE:HD12	1.86	0.41
1:D:160:VAL:CG1	1:D:161:GLY:N	2.84	0.41
1:D:195:TYR:CE2	1:D:200:ASP:HA	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ILE:HG13	1:D:404:VAL:HG21	2.03	0.41
1:D:434:ILE:HG13	1:D:442:VAL:HG22	2.02	0.41
1:D:482:LEU:HA	1:D:482:LEU:HD12	1.90	0.41
1:A:375:ILE:HD11	1:A:396:PHE:CZ	2.55	0.41
1:B:340:LEU:HA	1:B:340:LEU:HD23	1.88	0.41
1:D:240:PHE:CE1	1:D:737:ASP:HB3	2.55	0.41
1:D:330:TYR:HD1	1:D:337:TRP:CE2	2.38	0.41
1:D:475:PRO:HD3	1:D:557:THR:HB	2.01	0.41
1:D:72:GLN:C	1:D:74:ASN:N	2.74	0.41
1:A:124:TRP:HE3	1:A:124:TRP:HA	1.84	0.41
1:A:41:LYS:HE3	1:A:41:LYS:HB2	1.93	0.41
1:A:620:ASP:O	1:A:622:LYS:N	2.54	0.41
1:A:673:LEU:HD23	1:A:674:PRO:HD2	2.02	0.41
1:B:187:TRP:CZ3	1:B:281:ASN:OD1	2.73	0.41
1:B:293:MET:HE1	1:B:317:ARG:HG3	2.02	0.41
1:B:347:GLU:OE1	1:B:373:LYS:NZ	2.52	0.41
1:D:374:ILE:CD1	1:D:406:GLY:HA2	2.50	0.41
1:A:383:HIS:HA	1:A:404:VAL:HG23	2.03	0.41
1:A:457:TYR:CE1	1:A:472:CYS:HB2	2.56	0.41
1:B:563:TRP:CZ3	1:B:567:LEU:HD11	2.55	0.41
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.83	0.41
1:D:107:ILE:N	1:D:107:ILE:HD12	2.35	0.41
1:D:125:ARG:HG2	1:D:126:HIS:CD2	2.56	0.41
1:D:206:GLU:CD	1:D:666:TYR:HB2	2.41	0.41
1:D:258:LYS:O	1:D:259:ALA:C	2.59	0.41
1:D:422:TYR:C	1:D:424:GLY:H	2.24	0.41
1:D:520:ASN:C	1:D:522:THR:N	2.74	0.41
1:D:629:TRP:O	1:D:630:SER:CB	2.69	0.41
1:A:227:GLN:N	1:A:267:LYS:O	2.54	0.41
1:A:353:TRP:CZ2	1:A:670:TYR:HE1	2.38	0.41
1:B:135:TYR:O	1:B:137:LEU:N	2.54	0.41
1:B:660:GLU:OE2	1:B:684:ARG:NE	2.53	0.41
1:B:738:GLU:OE2	1:B:744:SER:HB2	2.21	0.41
1:C:175:LYS:HG3	1:C:182:SER:HB3	2.02	0.41
1:C:293:MET:HG2	1:C:315:TRP:CB	2.51	0.41
1:C:397:ILE:HG13	1:C:397:ILE:O	2.20	0.41
1:C:568:ALA:HA	1:C:573:ILE:O	2.21	0.41
1:C:82:GLU:HB2	1:C:467:TYR:OH	2.20	0.41
1:D:256:TYR:HA	1:D:257:PRO:HD3	1.92	0.41
1:A:343:ARG:HG2	1:A:389:ILE:HD12	2.02	0.41
1:A:415:LEU:CD2	1:A:415:LEU:C	2.89	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LYS:HE2	1:A:515:ASP:CB	2.51	0.41
1:B:524:PHE:CD2	1:B:580:GLY:HA2	2.56	0.41
1:B:644:SER:C	1:B:646:VAL:N	2.74	0.41
1:B:67:GLU:HA	1:B:79:PHE:O	2.20	0.41
1:C:188:THR:O	1:C:194:ILE:CG2	2.69	0.41
1:C:192:ASP:HA	1:C:195:TYR:OH	2.21	0.41
1:D:105:TYR:CD2	1:D:107:ILE:CD1	3.03	0.41
1:D:154:TRP:O	1:D:166:TYR:HA	2.21	0.41
1:D:581:ARG:NE	1:D:605:ASP:OD2	2.49	0.41
1:D:624:ILE:O	1:D:647:PHE:HA	2.21	0.41
1:A:132:TYR:CZ	1:A:155:VAL:HG12	2.56	0.41
1:A:387:PHE:CE2	1:A:394:CYS:CB	3.04	0.41
1:A:640:LEU:HB3	1:A:698:VAL:HG21	2.02	0.41
1:B:506:ASN:CG	1:B:506:ASN:O	2.59	0.41
1:B:599:GLY:N	1:B:602:GLU:OE1	2.46	0.41
1:C:248:TYR:O	1:C:249:PRO:C	2.59	0.41
1:C:622:LYS:C	1:C:623:ARG:HG3	2.41	0.41
1:D:387:PHE:CZ	1:D:394:CYS:SG	3.14	0.41
1:D:563:TRP:CZ3	1:D:567:LEU:HD11	2.56	0.41
1:D:732:ALA:O	1:D:733:MET:HB2	2.20	0.41
1:A:221:THR:HG23	1:A:274:ASP:OD2	2.21	0.41
1:B:308:GLN:C	1:B:309:GLU:HG3	2.41	0.41
1:C:82:GLU:HG2	1:C:83:TYR:CE1	2.56	0.41
1:D:148:ILE:O	1:D:149:PRO:C	2.59	0.41
1:D:146:GLU:HB3	1:D:180:LEU:C	2.42	0.41
1:A:180:LEU:O	1:A:181:PRO:O	2.39	0.40
1:A:341:VAL:C	1:A:343:ARG:H	2.24	0.40
1:B:501:ASP:O	1:B:505:GLN:HG2	2.21	0.40
1:B:594:ILE:CG2	1:B:601:PHE:HB2	2.51	0.40
1:B:659:TRP:O	1:B:667:THR:HG21	2.21	0.40
1:B:739:ASP:HB2	1:B:740:HIS:H	1.74	0.40
1:C:169:ASN:HD22	1:C:169:ASN:N	2.19	0.40
1:C:197:GLY:C	1:C:213:ALA:HB3	2.42	0.40
1:D:136:ASP:N	3:D:822:HOH:O	2.54	0.40
1:D:51:ASN:O	1:D:54:ARG:CD	2.69	0.40
1:D:623:ARG:HB3	1:D:763:PHE:CD1	2.56	0.40
1:D:258:LYS:NZ	1:D:661:TYR:O	2.52	0.40
1:A:107:ILE:HA	1:A:114:ILE:HA	2.02	0.40
1:A:158:SER:HB2	1:A:159:PRO:HD2	2.04	0.40
1:A:242:SER:CB	1:A:246:LEU:HD22	2.50	0.40
1:A:302:ASP:C	1:A:302:ASP:OD1	2.59	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:TYR:CZ	1:A:386:TYR:CE1	3.08	0.40
1:A:82:GLU:O	1:A:492:ARG:NH2	2.54	0.40
1:B:289:ALA:HB2	1:B:315:TRP:CE3	2.55	0.40
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.22	0.40
1:B:446:SER:HA	1:B:449:LEU:HG	2.01	0.40
1:B:550:PRO:O	1:B:551:CYS:CB	2.69	0.40
1:B:760:LYS:HD2	1:B:766:PRO:O	2.22	0.40
1:C:540:TYR:C	1:C:541:PRO:O	2.55	0.40
1:D:148:ILE:O	1:D:149:PRO:O	2.38	0.40
1:D:427:GLY:O	1:D:557:THR:HG23	2.21	0.40
1:D:627:TRP:CZ3	1:D:755:MET:HE1	2.56	0.40
1:D:720:SER:O	1:D:724:VAL:HG23	2.21	0.40
1:D:72:GLN:O	1:D:73:GLU:C	2.58	0.40
1:A:671:MET:SD	1:A:682:HIS:HD2	2.44	0.40
1:A:739:ASP:C	1:A:741:GLY:H	2.23	0.40
1:B:144:THR:O	1:B:147:ARG:HD2	2.21	0.40
1:B:356:ARG:HD3	1:B:585:TYR:HE1	1.85	0.40
1:B:433:LYS:HE2	1:B:488:ASP:OD1	2.21	0.40
1:B:470:LEU:HD23	1:B:470:LEU:HA	1.93	0.40
1:B:480:TYR:CD1	1:B:480:TYR:N	2.90	0.40
1:B:629:TRP:O	1:B:630:SER:CB	2.66	0.40
1:C:369:ASN:CA	1:C:389:ILE:HG23	2.51	0.40
1:C:70:TYR:HB3	1:C:79:PHE:HE2	1.87	0.40
1:D:504:LEU:HD22	1:D:509:MET:CE	2.52	0.40
1:A:602:GLU:N	1:A:602:GLU:OE2	2.50	0.40
1:B:744:SER:O	1:B:745:SER:C	2.59	0.40
1:B:82:GLU:OE1	1:B:82:GLU:HA	2.22	0.40
1:C:325:MET:CE	1:C:371:PHE:CE2	3.03	0.40
1:C:558:VAL:CG1	1:C:559:PHE:N	2.85	0.40
1:C:633:GLY:CA	1:C:655:PRO:HB3	2.46	0.40
1:C:741:GLY:O	1:C:742:ILE:C	2.59	0.40
1:C:753:THR:O	1:C:757:HIS:CD2	2.75	0.40
1:C:761:GLN:NE2	1:C:762:CYS:N	2.69	0.40
1:D:110:ASP:C	1:D:112:GLN:N	2.71	0.40
1:D:87:SER:O	1:D:88:VAL:C	2.59	0.40
1:D:90:LEU:HA	1:D:90:LEU:HD12	1.89	0.40
1:A:126:HIS:CD2	1:A:209:SER:C	2.95	0.40
1:A:83:TYR:C	1:A:492:ARG:NH2	2.75	0.40
1:A:649:CYS:HB3	1:A:699:GLU:HB2	2.01	0.40
1:B:121:VAL:HB	1:B:129:THR:OG1	2.22	0.40
1:B:199:THR:HG23	1:B:213:ALA:HB2	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:ARG:HE	1:B:687:THR:HG21	1.87	0.40
1:C:657:SER:HB3	1:C:719:ILE:CD1	2.51	0.40
1:C:743:ALA:O	1:C:744:SER:C	2.60	0.40
1:D:383:HIS:HB3	1:D:398:THR:OG1	2.20	0.40
1:D:50:LYS:HD3	1:D:50:LYS:HA	1.80	0.40
1:D:642:SER:O	1:D:643:GLY:C	2.60	0.40
1:D:77:LEU:CD1	1:D:77:LEU:N	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/728 (100%)	593 (82%)	112 (15%)	21 (3%)	4	24
1	B	726/728 (100%)	622 (86%)	84 (12%)	20 (3%)	5	25
1	C	726/728 (100%)	620 (85%)	86 (12%)	20 (3%)	5	25
1	D	726/728 (100%)	634 (87%)	73 (10%)	19 (3%)	5	26
All	All	2904/2912 (100%)	2469 (85%)	355 (12%)	80 (3%)	5	25

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	320	GLN
1	A	439	TYR
1	B	137	LEU
1	B	320	GLN
1	B	520	ASN
1	B	712	HIS
1	C	74	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	106	SER
1	C	143	ILE
1	C	548	ALA
1	D	88	VAL
1	D	111	GLY
1	D	320	GLN
1	A	139	LYS
1	A	143	ILE
1	A	181	PRO
1	A	209	SER
1	A	261	ALA
1	A	389	ILE
1	A	614	SER
1	A	621	ASN
1	B	73	GLU
1	B	146	GLU
1	B	280	THR
1	B	536	LYS
1	B	764	SER
1	C	712	HIS
1	D	138	ASN
1	D	764	SER
1	A	231	THR
1	A	242	SER
1	A	577	SER
1	B	377	ASN
1	B	616	MET
1	C	583	SER
1	C	668	GLU
1	D	149	PRO
1	D	366	LEU
1	D	521	GLU
1	D	710	ASN
1	D	712	HIS
1	A	51	ASN
1	A	74	ASN
1	A	149	PRO
1	A	333	SER
1	A	491	LEU
1	B	261	ALA
1	C	366	LEU
1	C	536	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	695	PHE
1	D	178	PRO
1	D	423	LYS
1	D	683	TYR
1	A	191	GLU
1	A	447	CYS
1	B	136	ASP
1	B	143	ILE
1	B	548	ALA
1	C	51	ASN
1	C	218	PRO
1	C	259	ALA
1	C	320	GLN
1	C	664	SER
1	C	667	THR
1	C	715	GLN
1	C	737	ASP
1	D	130	ALA
1	D	714	GLN
1	B	645	GLY
1	B	714	GLN
1	D	143	ILE
1	D	280	THR
1	B	109	PRO
1	B	674	PRO
1	B	742	ILE
1	D	742	ILE
1	C	355	GLY
1	C	541	PRO
1	D	181	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	653/653 (100%)	610 (93%)	43 (7%)	16 47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	653/653 (100%)	624 (96%)	29 (4%)	28	61
1	C	653/653 (100%)	616 (94%)	37 (6%)	20	52
1	D	653/653 (100%)	616 (94%)	37 (6%)	20	52
All	All	2612/2612 (100%)	2466 (94%)	146 (6%)	21	52

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	57	LEU
1	A	77	LEU
1	A	95	PHE
1	A	96	ASP
1	A	106	SER
1	A	109	PRO
1	A	133	ASP
1	A	145	GLU
1	A	147	ARG
1	A	170	ASN
1	A	186	THR
1	A	202	VAL
1	A	214	LEU
1	A	243	ASP
1	A	254	VAL
1	A	256	TYR
1	A	279	VAL
1	A	280	THR
1	A	288	THR
1	A	293	MET
1	A	339	CYS
1	A	385	CYS
1	A	388	GLN
1	A	389	ILE
1	A	391	LYS
1	A	393	ASP
1	A	413	ASP
1	A	458	SER
1	A	507	VAL
1	A	536	LYS
1	A	566	TYR
1	A	570	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	577	SER
1	A	597	ARG
1	A	621	ASN
1	A	657	SER
1	A	658	ARG
1	A	677	GLU
1	A	683	TYR
1	A	704	HIS
1	A	714	GLN
1	A	728	VAL
1	B	54	ARG
1	B	72	GLN
1	B	73	GLU
1	B	74	ASN
1	B	75	ASN
1	B	89	PHE
1	B	91	GLU
1	B	108	SER
1	B	145	GLU
1	B	214	LEU
1	B	239	SER
1	B	243	ASP
1	B	254	VAL
1	B	272	ASN
1	B	277	SER
1	B	283	THR
1	B	332	GLU
1	B	341	VAL
1	B	382	ARG
1	B	448	GLU
1	B	452	GLU
1	B	487	ASN
1	B	522	THR
1	B	546	VAL
1	B	606	GLN
1	B	658	ARG
1	B	677	GLU
1	B	700	TYR
1	B	761	GLN
1	C	96	ASP
1	C	108	SER
1	C	118	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	125	ARG
1	C	133	ASP
1	C	145	GLU
1	C	170	ASN
1	C	184	ARG
1	C	214	LEU
1	C	215	TRP
1	C	254	VAL
1	C	256	TYR
1	C	293	MET
1	C	301	CYS
1	C	319	ILE
1	C	326	ASP
1	C	329	ASP
1	C	333	SER
1	C	336	ARG
1	C	382	ARG
1	C	385	CYS
1	C	388	GLN
1	C	401	THR
1	C	448	GLU
1	C	472	CYS
1	C	492	ARG
1	C	539	LYS
1	C	546	VAL
1	C	566	TYR
1	C	583	SER
1	C	621	ASN
1	C	627	TRP
1	C	658	ARG
1	C	663	ASP
1	C	728	VAL
1	C	761	GLN
1	C	764	SER
1	D	52	THR
1	D	55	LEU
1	D	57	LEU
1	D	63	ILE
1	D	80	ASN
1	D	85	ASN
1	D	113	PHE
1	D	121	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	125	ARG
1	D	137	LEU
1	D	138	ASN
1	D	151	ASN
1	D	156	THR
1	D	158	SER
1	D	169	ASN
1	D	180	LEU
1	D	184	ARG
1	D	191	GLU
1	D	214	LEU
1	D	221	THR
1	D	254	VAL
1	D	256	TYR
1	D	272	ASN
1	D	278	SER
1	D	284	SER
1	D	351	THR
1	D	385	CYS
1	D	393	ASP
1	D	448	GLU
1	D	487	ASN
1	D	492	ARG
1	D	566	TYR
1	D	606	GLN
1	D	677	GLU
1	D	681	ASP
1	D	685	ASN
1	D	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	123	GLN
1	A	126	HIS
1	A	141	GLN
1	A	169	ASN
1	A	170	ASN
1	A	263	ASN
1	A	286	GLN
1	A	314	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	345	HIS
1	A	388	GLN
1	A	505	GLN
1	A	572	ASN
1	A	595	ASN
1	A	621	ASN
1	A	712	HIS
1	A	731	GLN
1	A	757	HIS
1	B	51	ASN
1	B	66	HIS
1	B	74	ASN
1	B	75	ASN
1	B	123	GLN
1	B	169	ASN
1	B	272	ASN
1	B	281	ASN
1	B	314	GLN
1	B	435	GLN
1	B	487	ASN
1	B	506	ASN
1	B	712	HIS
1	B	731	GLN
1	B	748	HIS
1	B	761	GLN
1	C	75	ASN
1	C	103	ASN
1	C	123	GLN
1	C	126	HIS
1	C	138	ASN
1	C	169	ASN
1	C	170	ASN
1	C	345	HIS
1	C	572	ASN
1	C	621	ASN
1	C	712	HIS
1	C	731	GLN
1	C	757	HIS
1	D	72	GLN
1	D	74	ASN
1	D	92	ASN
1	D	123	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	150	ASN
1	D	169	ASN
1	D	227	GLN
1	D	272	ASN
1	D	286	GLN
1	D	314	GLN
1	D	435	GLN
1	D	455	GLN
1	D	487	ASN
1	D	506	ASN
1	D	595	ASN
1	D	685	ASN
1	D	712	HIS
1	D	714	GLN
1	D	731	GLN
1	D	761	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	13Z	D	767	1	23,27,27	1.08	2 (8%)	25,41,41	2.15	3 (12%)
2	13Z	B	767	1	23,27,27	1.25	2 (8%)	25,41,41	2.15	3 (12%)
2	13Z	C	767	1	23,27,27	1.53	2 (8%)	25,41,41	1.94	3 (12%)
2	13Z	A	767	1	23,27,27	1.48	4 (17%)	25,41,41	2.26	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	13Z	D	767	1	-	7/20/39/39	0/2/2/2
2	13Z	B	767	1	-	5/20/39/39	0/2/2/2
2	13Z	C	767	1	-	4/20/39/39	0/2/2/2
2	13Z	A	767	1	-	7/20/39/39	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	767	13Z	C7-C1	5.76	1.60	1.54
2	B	767	13Z	C7-C1	4.08	1.59	1.54
2	A	767	13Z	C7-C1	4.07	1.58	1.54
2	A	767	13Z	C11-N4	3.94	1.53	1.49
2	D	767	13Z	C7-C1	3.47	1.58	1.54
2	A	767	13Z	C1-N1	2.36	1.50	1.47
2	C	767	13Z	C5-N1	2.23	1.42	1.35
2	B	767	13Z	C5-N1	2.16	1.41	1.35
2	D	767	13Z	C1-N1	2.08	1.49	1.47
2	A	767	13Z	C5-N1	2.08	1.41	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	767	13Z	C10-C9-N3	9.60	131.23	120.51
2	B	767	13Z	C10-C9-N3	8.87	130.41	120.51
2	D	767	13Z	C10-C9-N3	8.78	130.31	120.51
2	C	767	13Z	C10-C9-N3	7.88	129.30	120.51
2	D	767	13Z	C8-C7-C1	4.22	117.96	110.02
2	B	767	13Z	C8-C7-C1	4.15	117.83	110.02
2	A	767	13Z	C8-C7-C1	3.37	116.36	110.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	767	13Z	C8-C7-C1	2.94	115.56	110.02
2	D	767	13Z	C4-N1-C5	-2.49	124.37	129.33
2	C	767	13Z	C4-N1-C5	-2.46	124.42	129.33
2	B	767	13Z	C4-N1-C5	-2.12	125.09	129.33
2	A	767	13Z	C2-C1-N1	2.04	104.77	101.71

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	767	13Z	C13-C11-N4-C6
2	D	767	13Z	C15-C11-N4-C6
2	D	767	13Z	C17-C11-N4-C6
2	D	767	13Z	N4-C11-C15-O4
2	D	767	13Z	C13-C11-C15-O4
2	D	767	13Z	C17-C11-C15-O4
2	B	767	13Z	C15-C11-N4-C6
2	C	767	13Z	C13-C11-N4-C6
2	C	767	13Z	C15-C11-N4-C6
2	C	767	13Z	C17-C11-N4-C6
2	A	767	13Z	C5-C6-N4-C11
2	A	767	13Z	C13-C11-N4-C6
2	A	767	13Z	C15-C11-N4-C6
2	A	767	13Z	C17-C11-N4-C6
2	A	767	13Z	N4-C11-C15-O4
2	A	767	13Z	C13-C11-C15-O4
2	A	767	13Z	C17-C11-C15-O4
2	B	767	13Z	O1-C5-C6-N4
2	B	767	13Z	N1-C5-C6-N4
2	D	767	13Z	C5-C6-N4-C11
2	B	767	13Z	C5-C6-N4-C11
2	C	767	13Z	C5-C6-N4-C11
2	B	767	13Z	C17-C11-N4-C6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

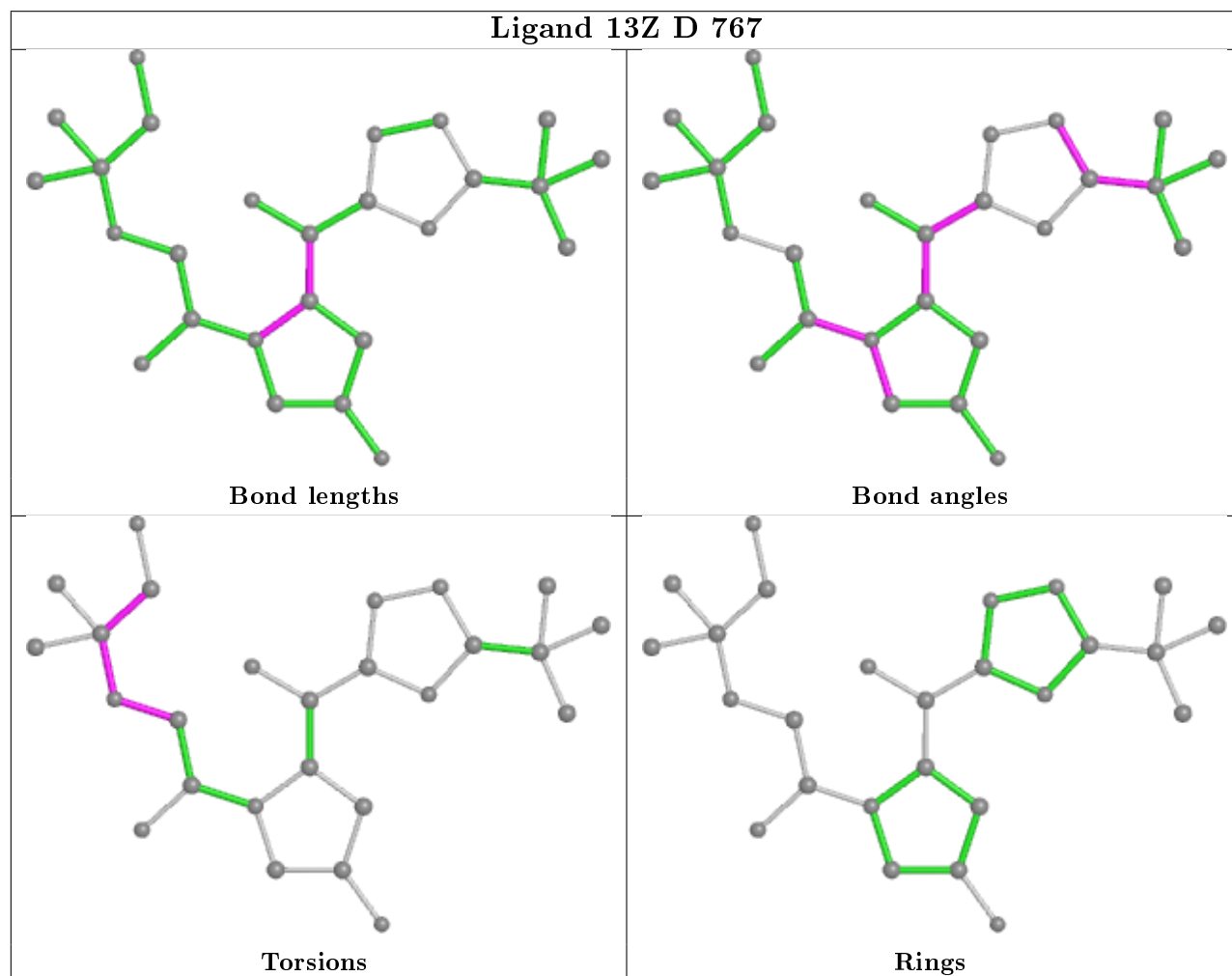
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	767	13Z	3	0
2	B	767	13Z	2	0
2	C	767	13Z	1	0

*Continued on next page...*

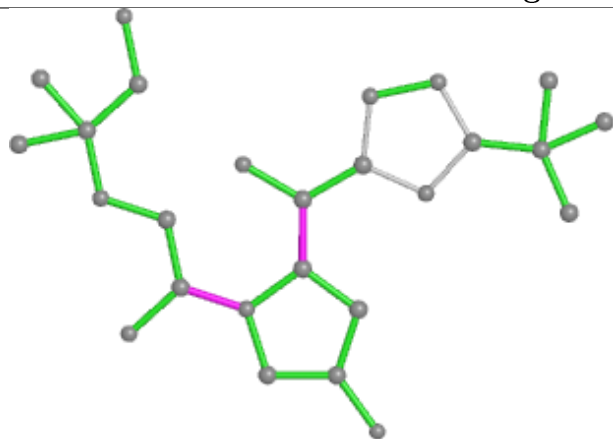
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	767	13Z	2	0

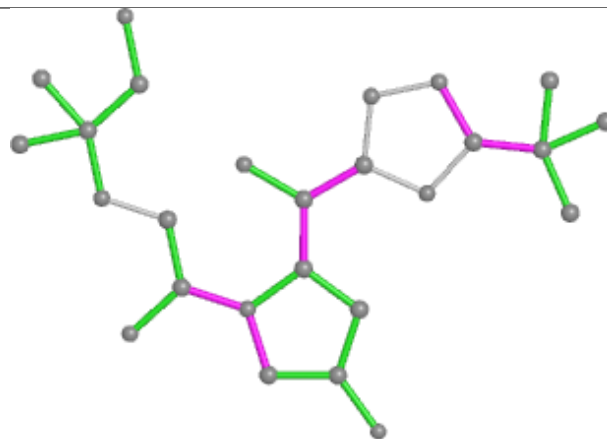
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



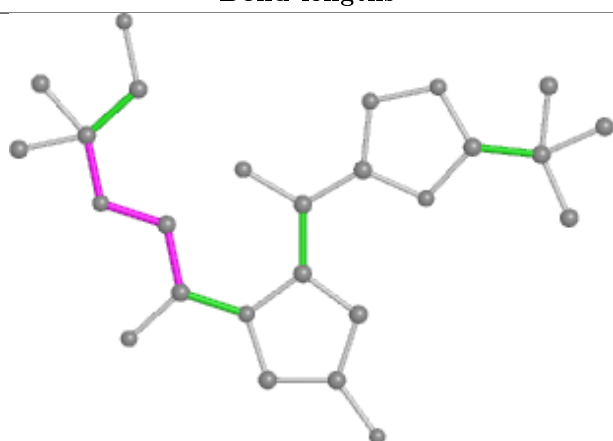
## Ligand 13Z B 767



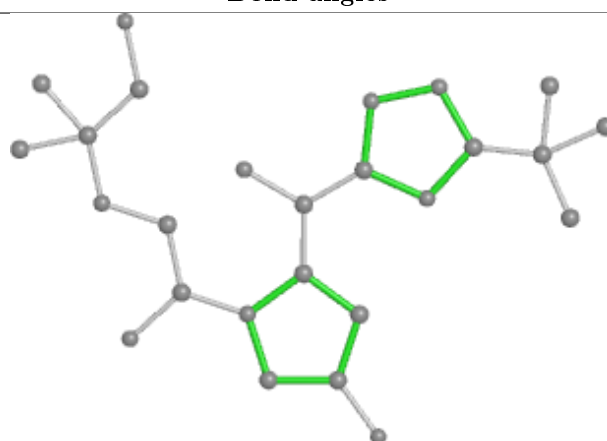
Bond lengths



Bond angles

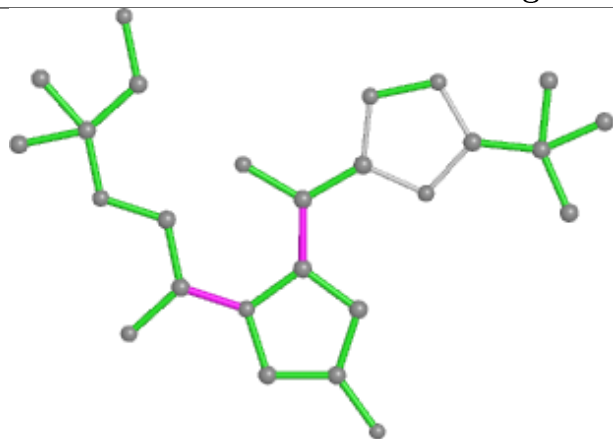


Torsions

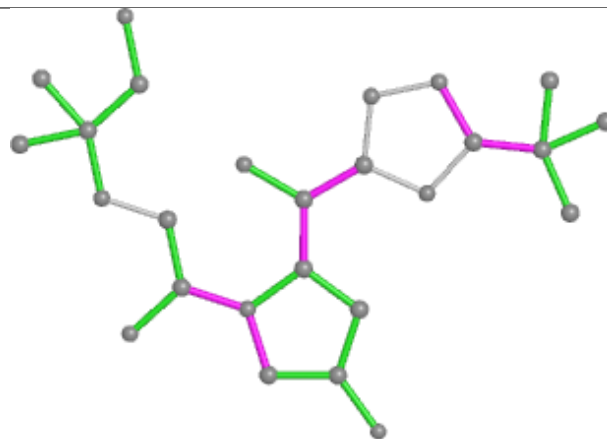


Rings

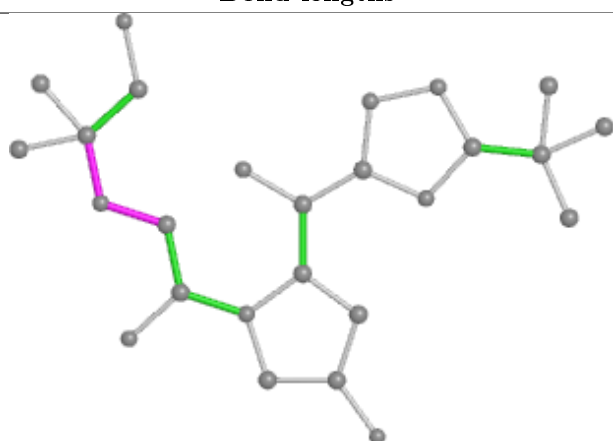
## Ligand 13Z C 767



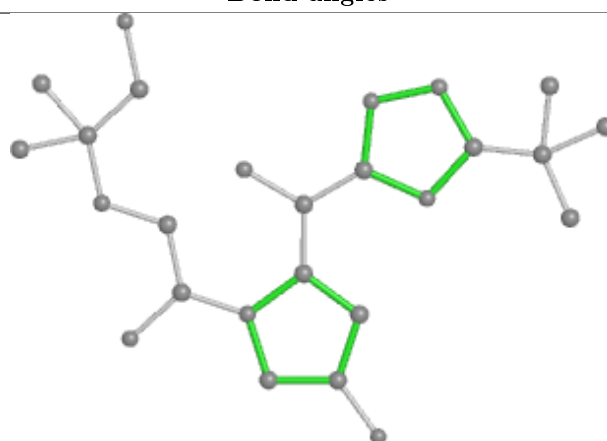
Bond lengths



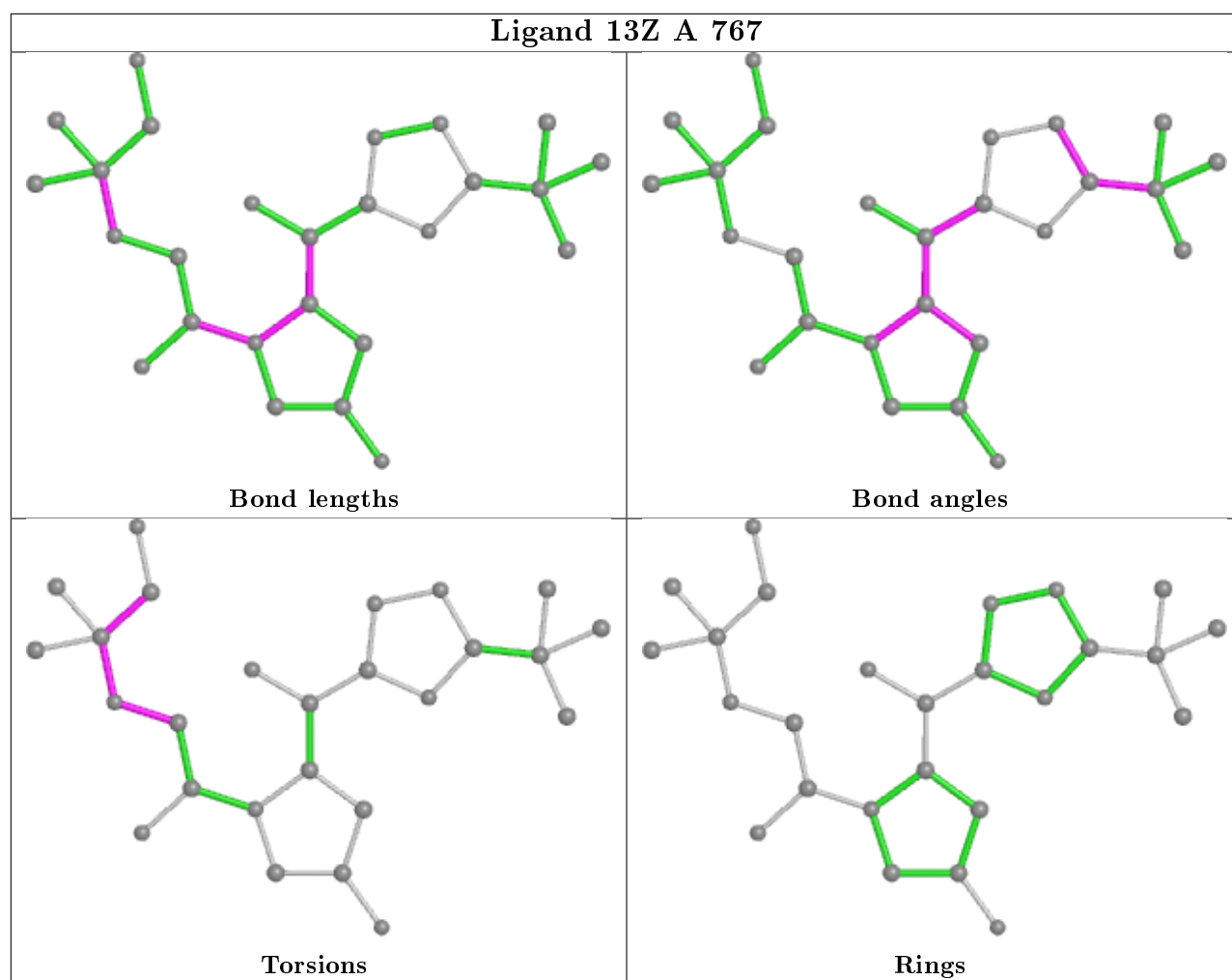
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.